# ME 471: TURBULENT COMBUSTION

J. Urzay




Spring 2012

**PROFESSOR RICHARD FEYNMAN'S LECTURES**

# *" FIRE "*



(Movie)

STANFORD MECHANICAL ENGINEERING

# ME 471: TURBULENT COMBUSTION

**Spring 2012**

**Instructor:** Javier Urzay, Ph.D.

E-mail: jurzay@stanford.edu

Office: 206 CTR, Phone: 650 723 9601.

Office Hours: Mondays 9:00 AM-11:00 AM.

**Lectures:** Tuesdays and Thursdays, 10:00 AM-11:15 AM at room 240-101.

**Textbooks**:

- N. Peters, "Turbulent combustion", Cambridge University Press, 2005.
- R.S. Cant & E. Mastorakos, "An introduction to turbulent reacting flows", Imperial College Press, 2008.
- F.A. Williams, "Combustion Theory", Benjamin Cummins, 1985.

Supplementary material shall be provided in class.

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# ME 471: TURBULENT COMBUSTION

## Spring 2012

**Homeworks:** There will be 4 homework assignments. Homework will be assigned bi-weekly on Thursdays and collected on Tuesdays two weeks later at the beginning of the lecture, as detailed in the course schedule. No late homeworks will be accepted.

**Exams:** Midterm Exam: Tuesday, May 15, in class.

Final Exam: Tuesday, June 12, location TBA.

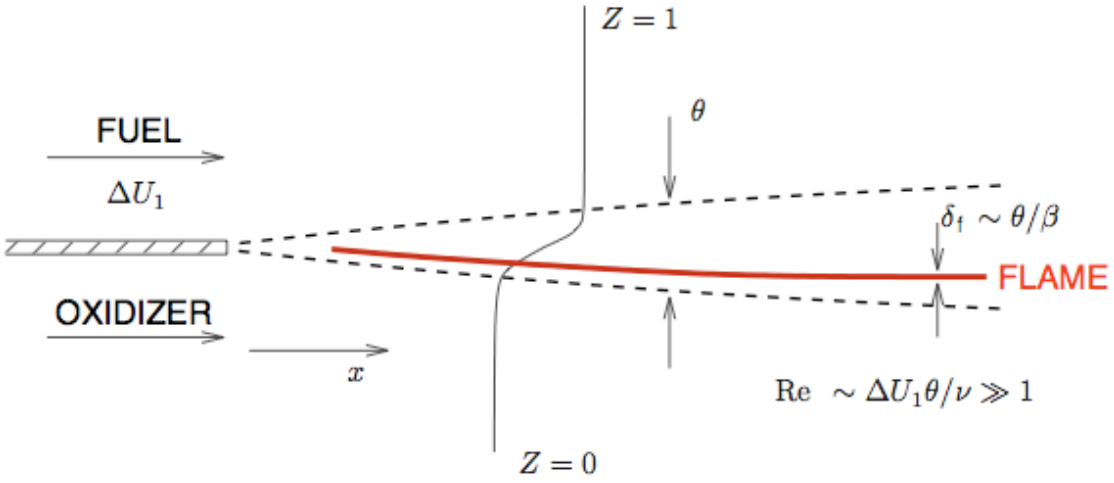
Both exams will consist of two parts: i) Short Questions (closed books, closed notes, no calculator), and ii) Problems (open book and open notes, calculator allowed).

**Grading Scheme:** 20% Homeworks + 35% Midterm Exam + 45% Final Exam.

**Academic Integrity:**. The Stanford Honor Code will be followed.
http://www.stanford.edu/dept/vpsa/judicialaffairs/guiding/honorcode.htm

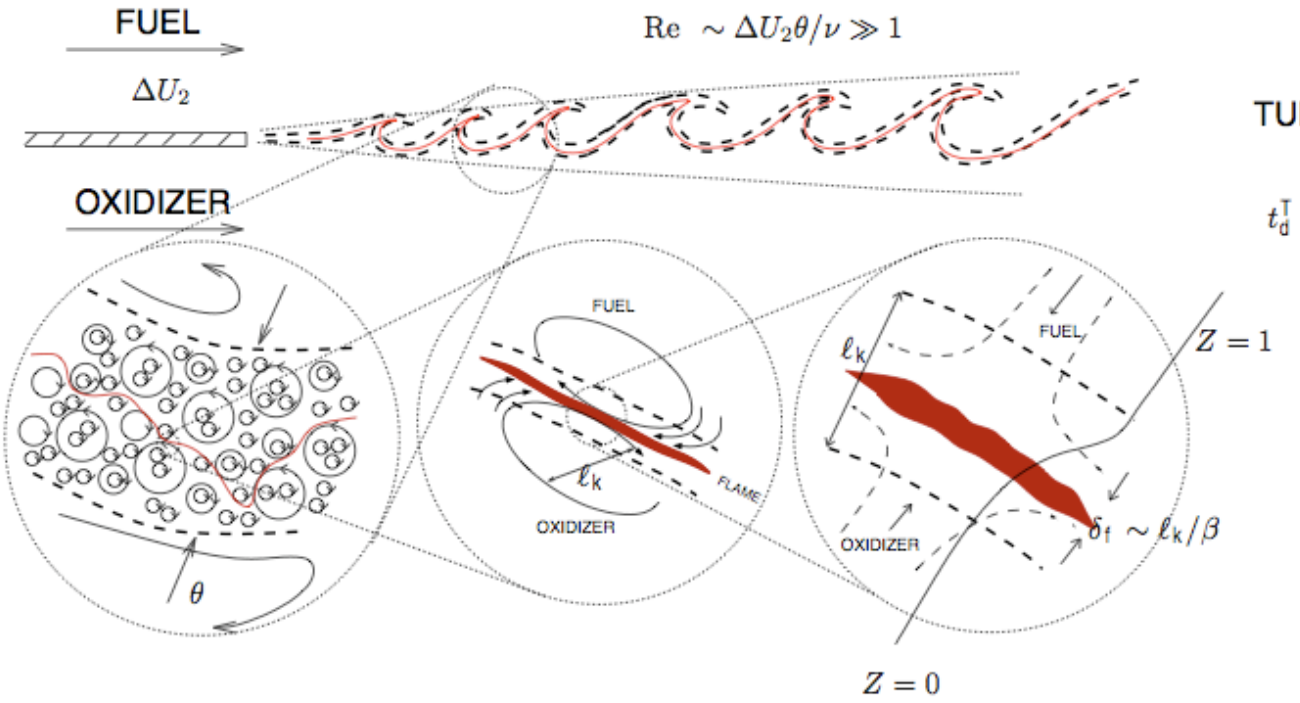
**Website:** http://www.stanford.edu/~jurzay/ME_471

# The turbulent-combustion problematique




LAMINAR MIXING LAYER

$$t_d^L \sim \theta^2/D_F$$



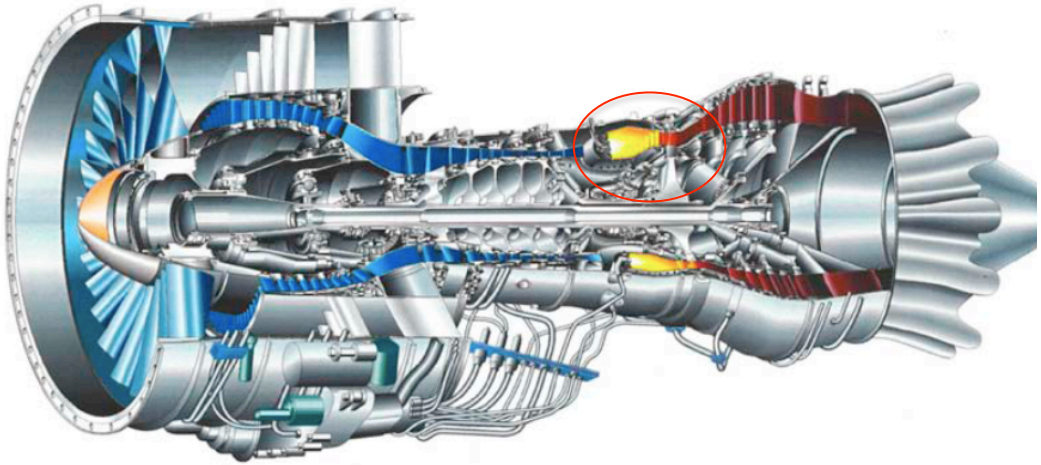

TURBULENT MIXING LAYER

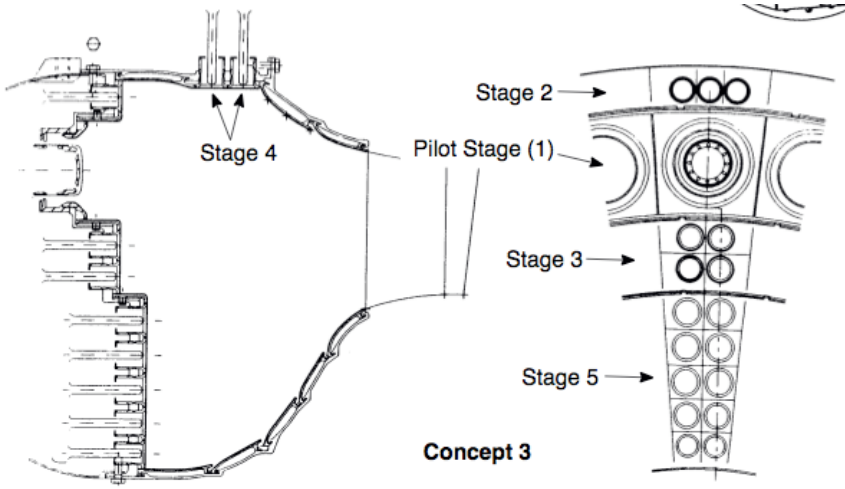
$$t_d^T \sim \ell_k^2/D_F \sim t_d^L \mathrm{Re}^{-1/2} \ll t_d^L$$

$$t_l \sim \theta/\Delta U_2 \gg t_d^T$$

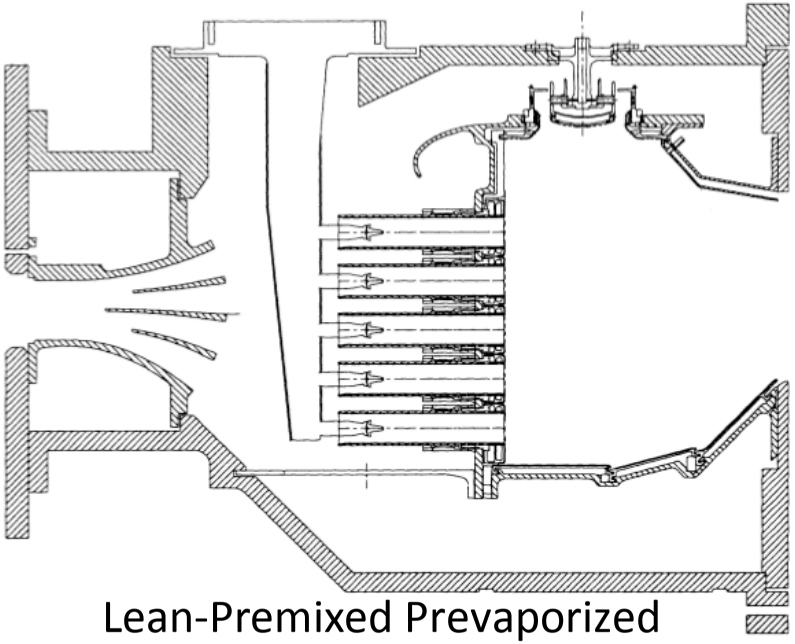
# Combustion engineering

## 1. GAS TURBINES

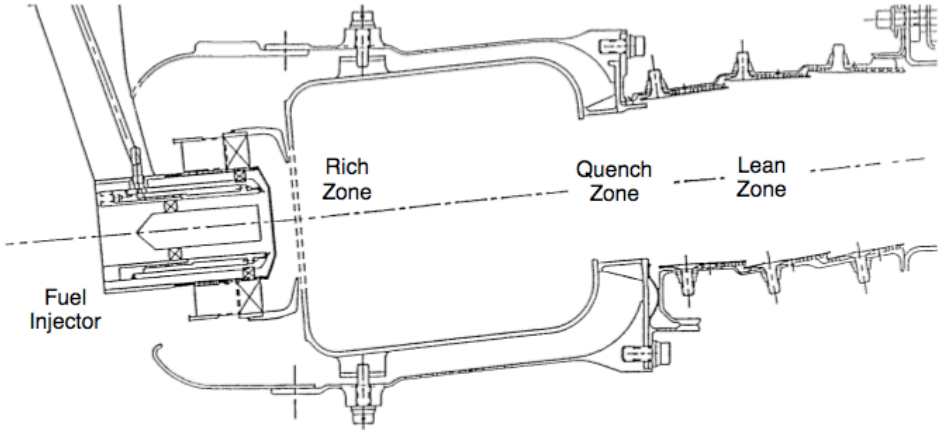





Lean-Direct Injection



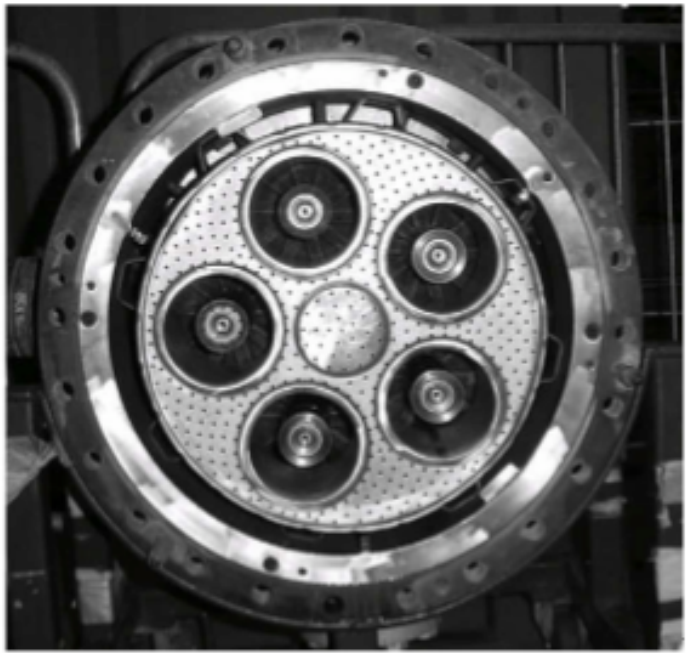
Lean-Premixed Prevaporized

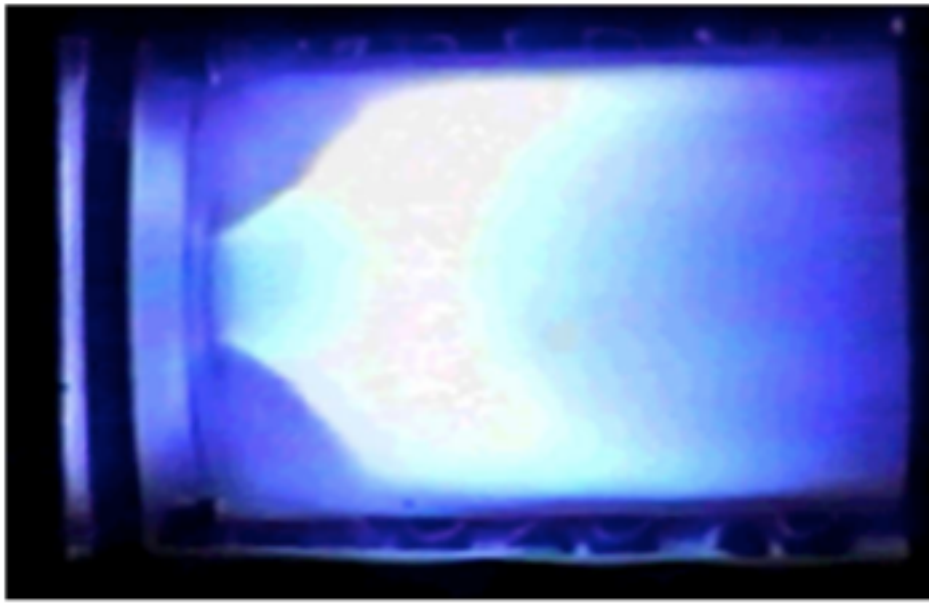


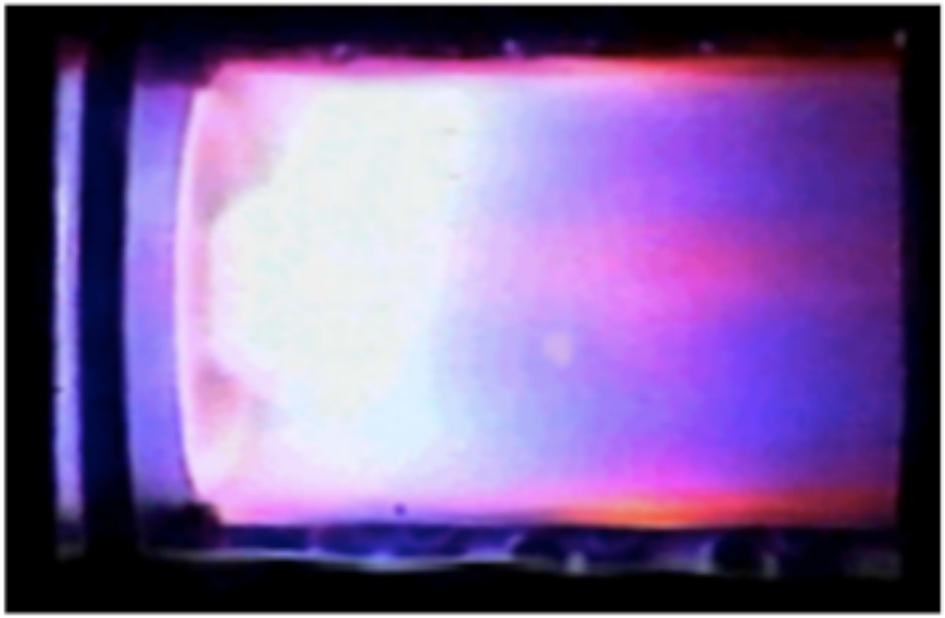

Rich/Quench/Lean

# Combustion engineering









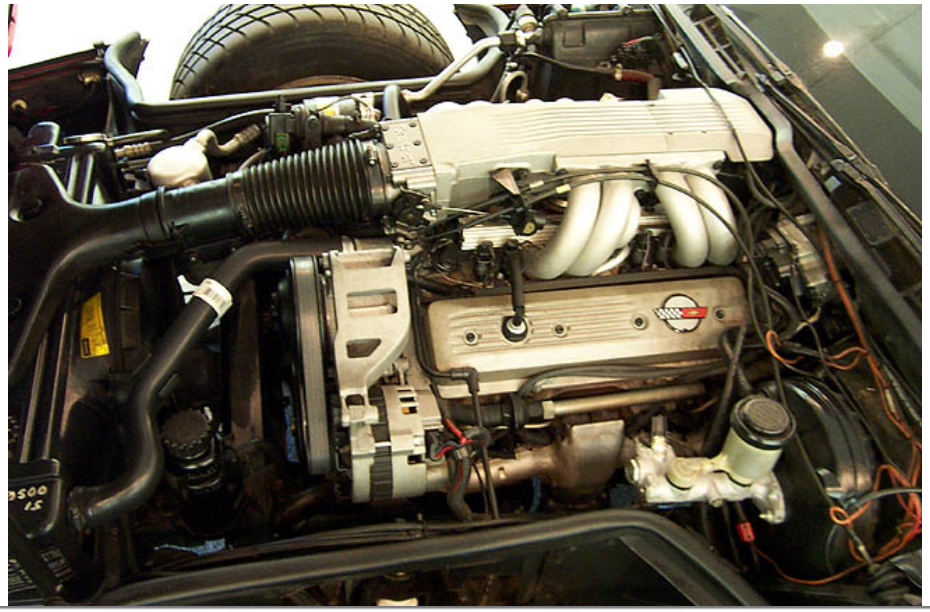


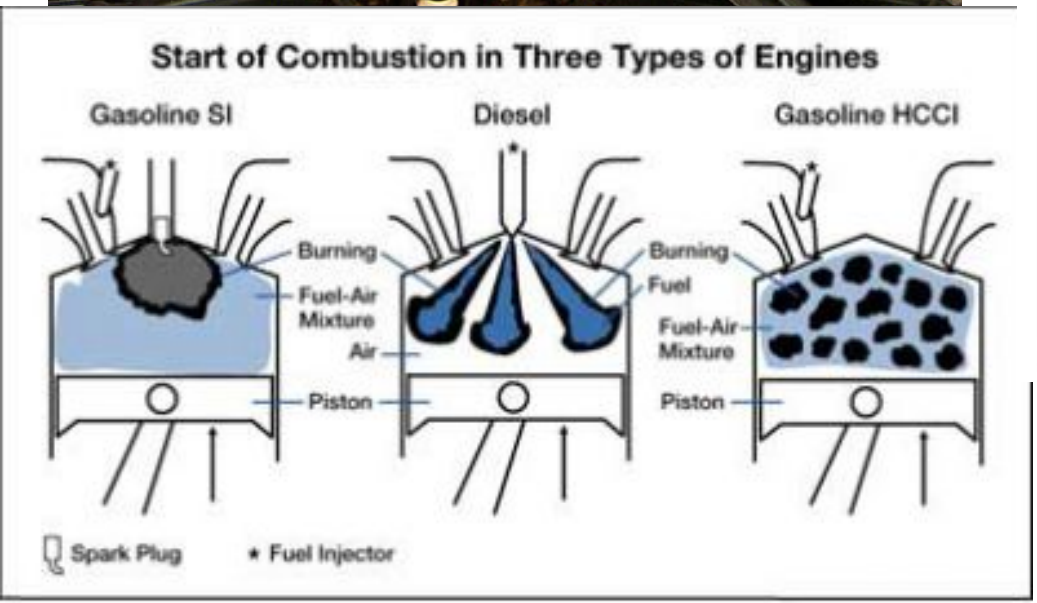
Ignition in a helicopter combustor
(Credits: Turbomeca)

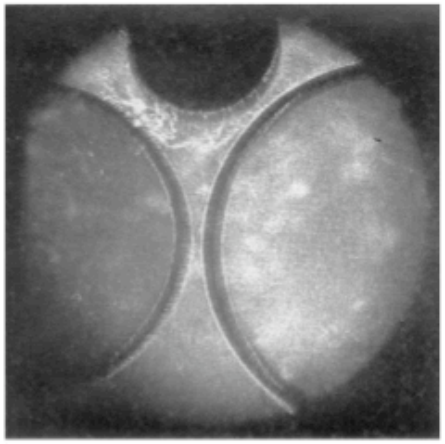
(Movie)

# Combustion in propulsion engineering

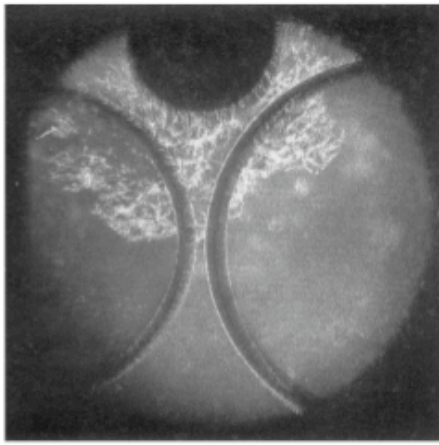
## 2. INTERNAL COMBUSTION ENGINES



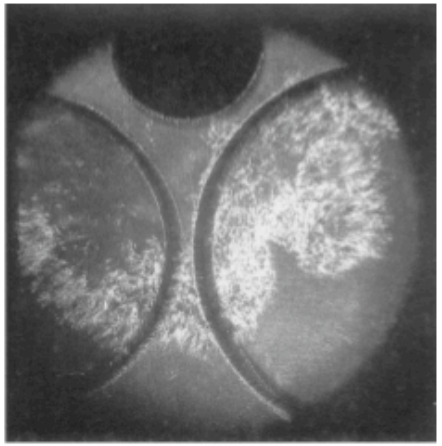


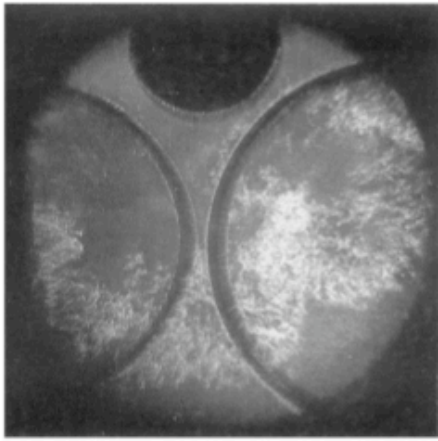
22°bTDC



14°bTDC



4°bTDC



TDC

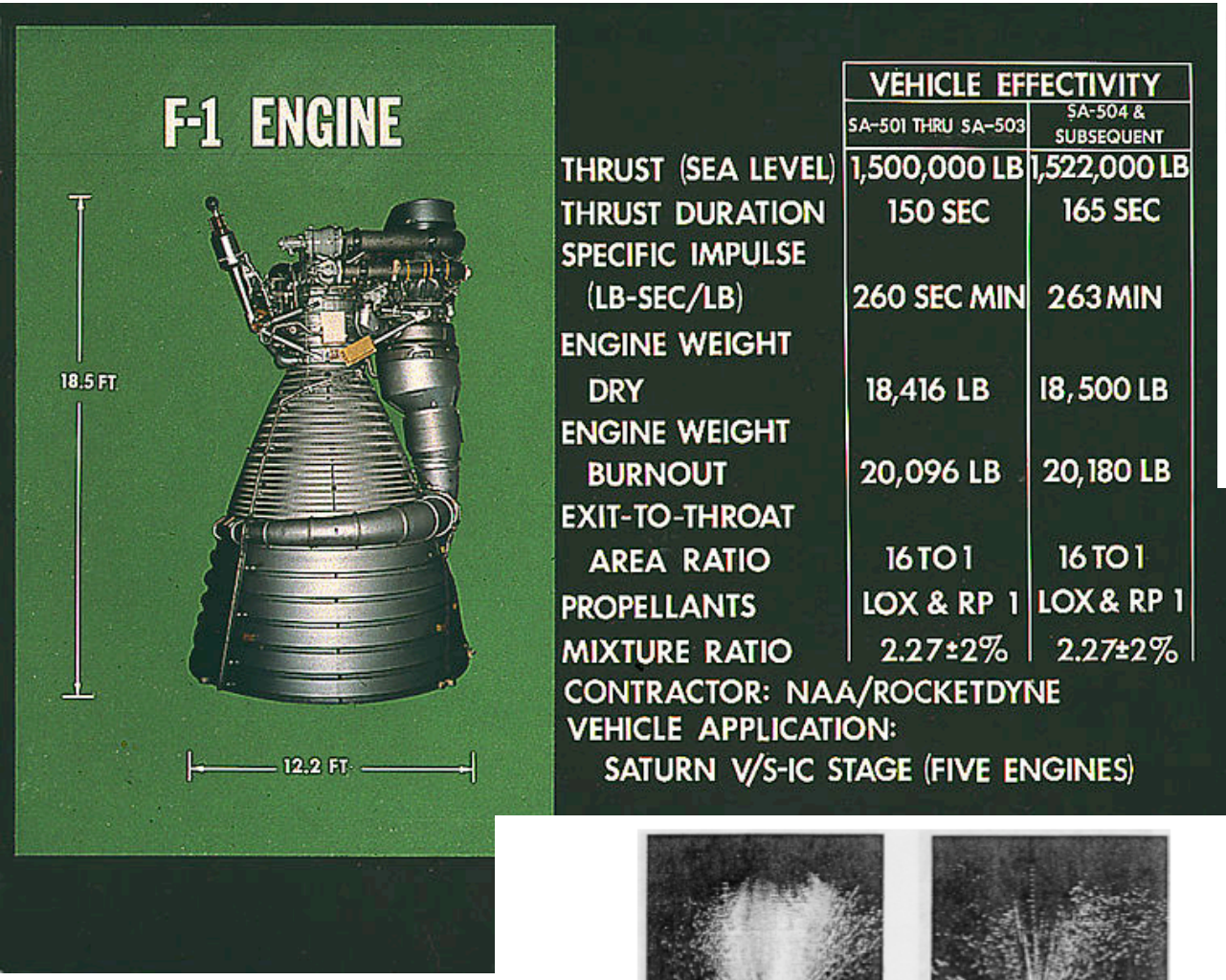


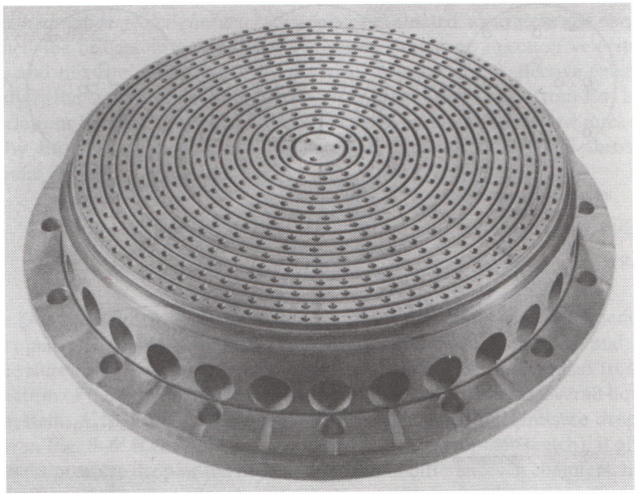
Spark-ignition engine, in-cylinder video

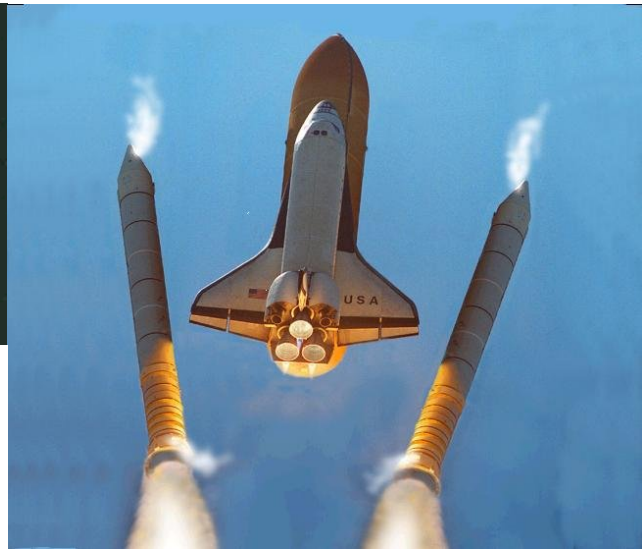
(Movie)

# Combustion in propulsion engineering

## 3. ROCKET PROPULSION



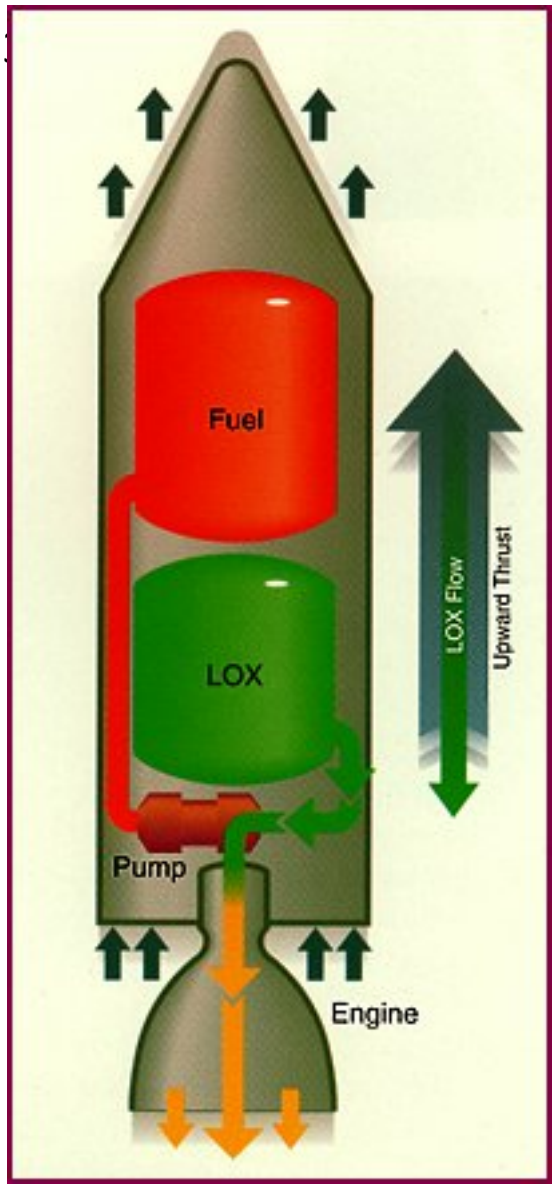


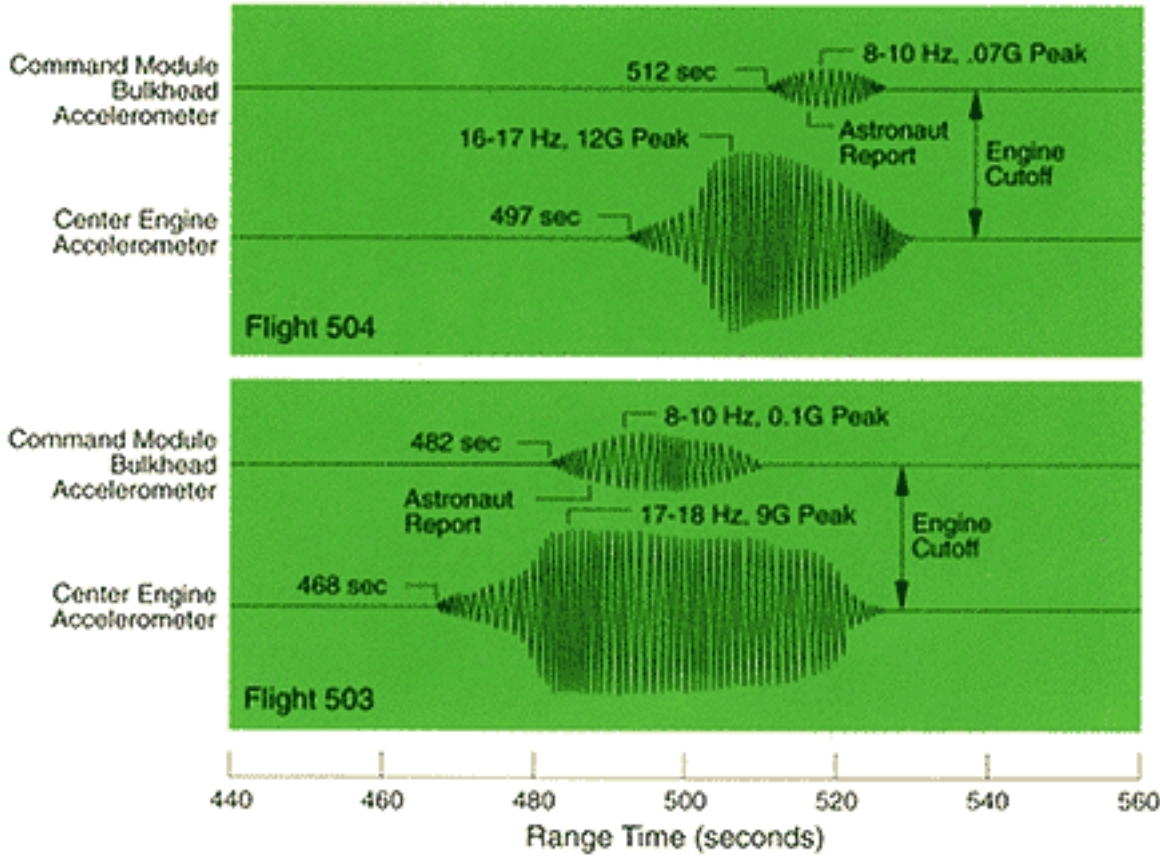



(a) (b)

. Spray patterns of non-gelled (a) and gelled water (b) using a triplet injector

# Combustion in propulsion engineering




Data recorded from on-board accelerometers on the Apollo 6 and 8 missions showed pogo as measured at the center engine mount and the response at the crew module. Credits: NASA



SATURN V, 1st STAGE (F-1) STATIC TESTS
STENNIS SPACE CENTER (MISSISSIPPI TEST FACILITY)
Credits: NASA

(Movie)

# Combustion engineering

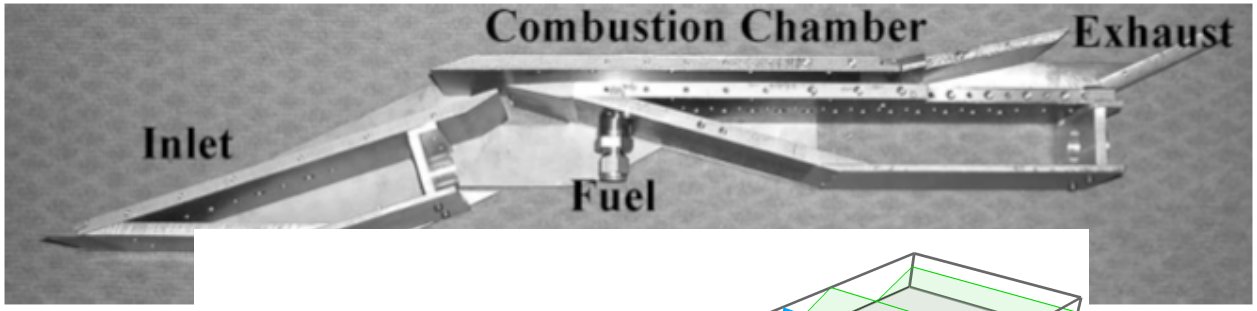
4. SUPERSONIC AIR-BREATHING PROPULSION

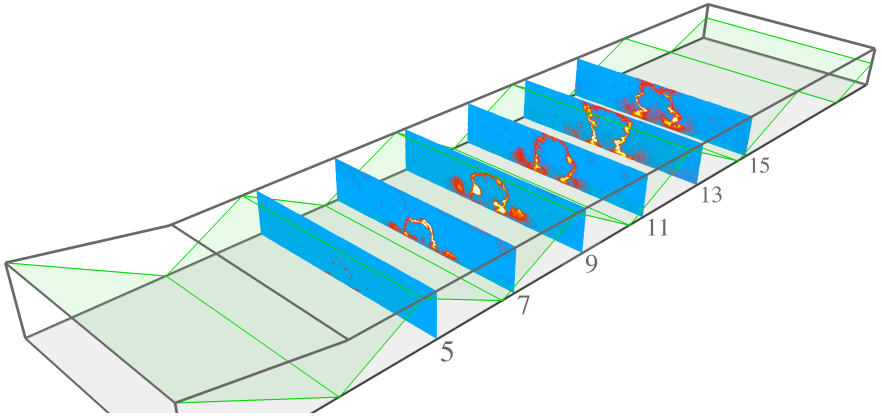


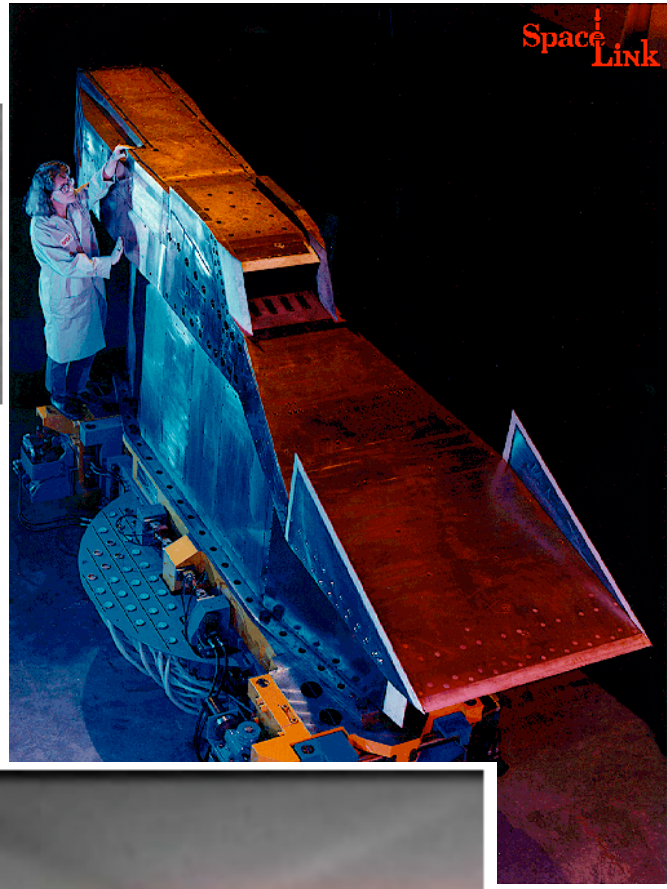
**X-51, Mach 4.5 to 7**



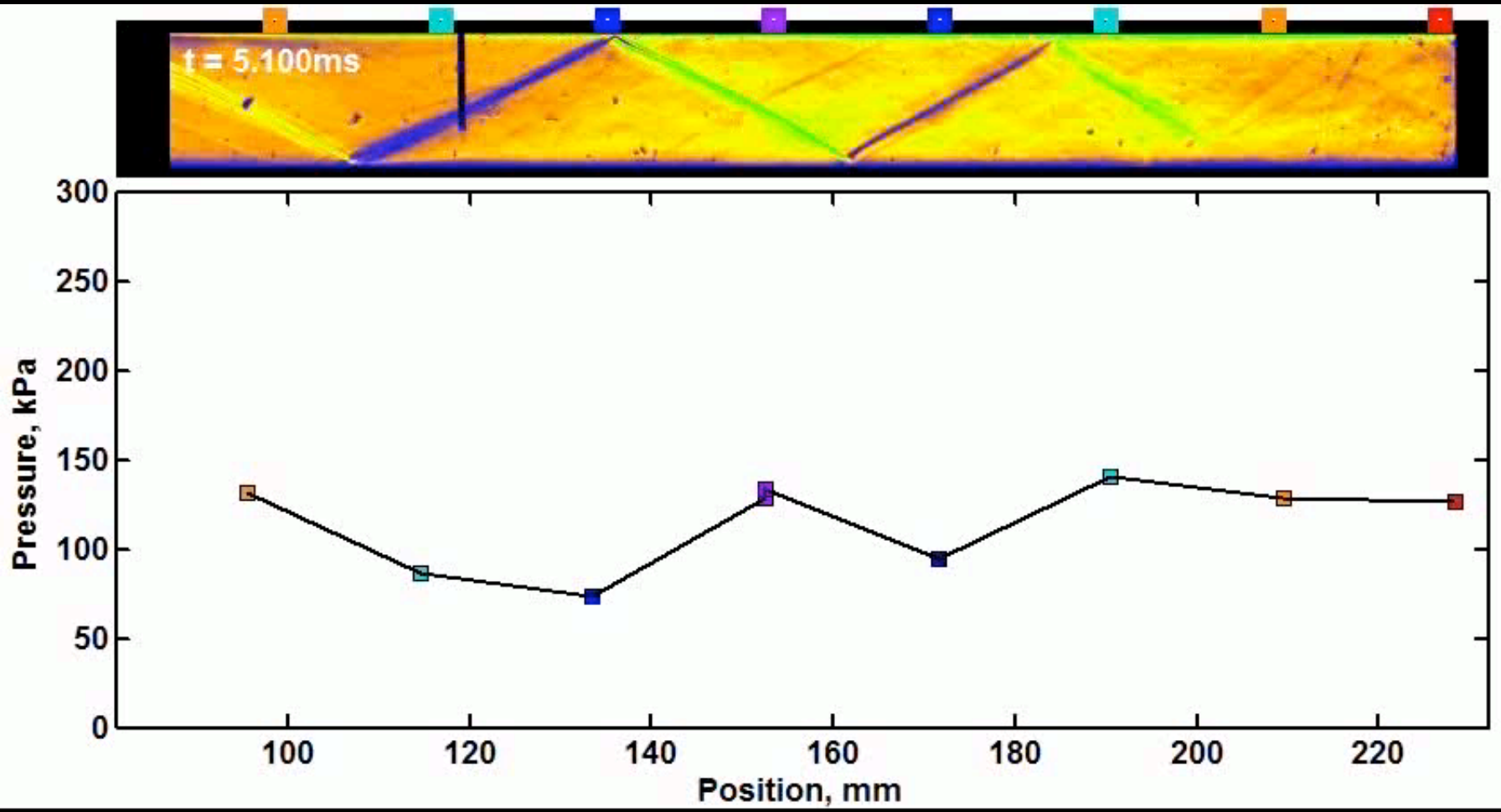

**Hyper-X, Mach 10**





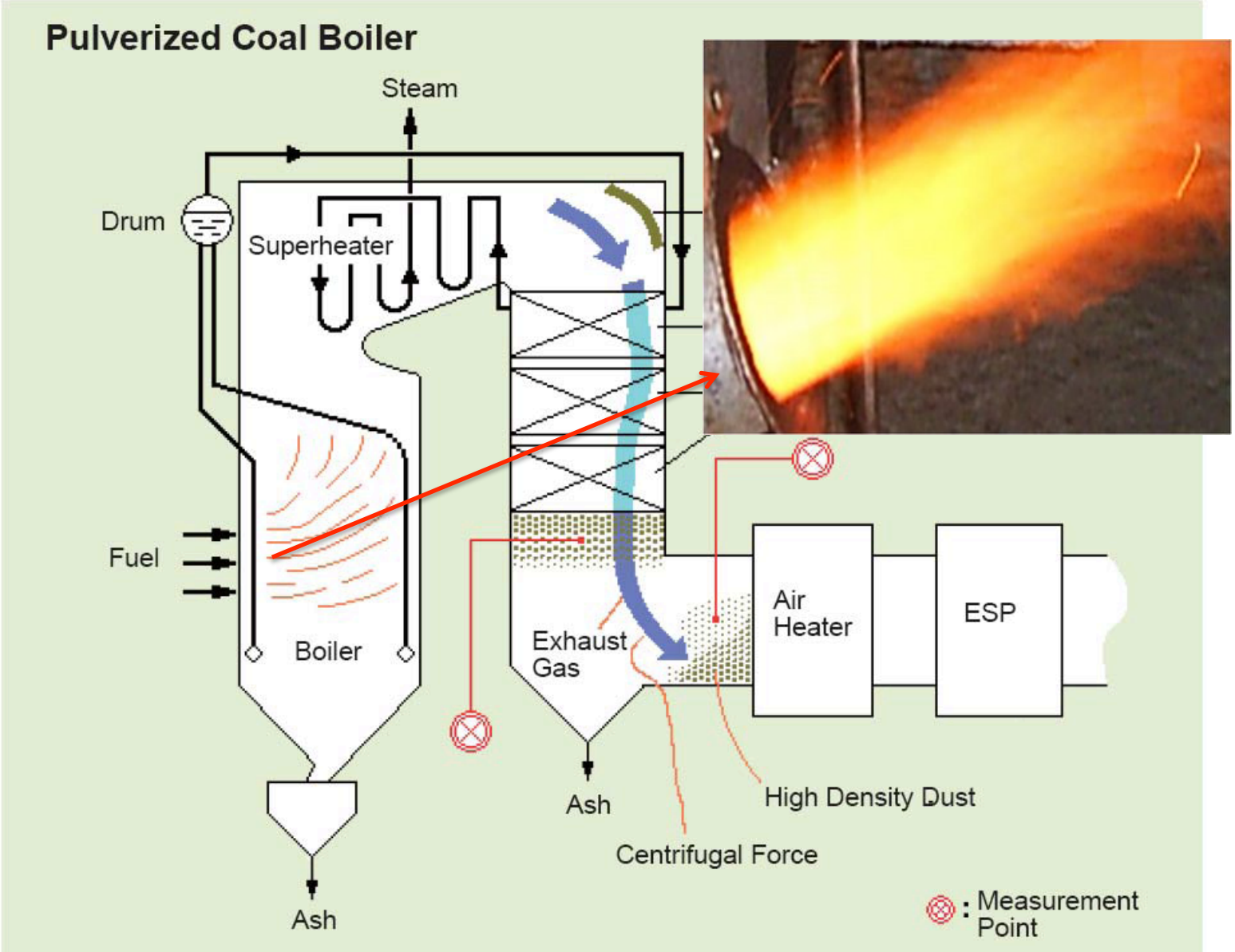




CESCO Experiment
Credits: Dr. Mirko Gamba (Stanford)

(Movie)

# Combustion engineering

5. PULVERIZED COAL FURNACES



Pulverized coal fired through a
$CH_4$-Air premixed flame (12000 fps)
Credits: firescience.com



(Movie)

# Combustion engineering

6. Fire Protection









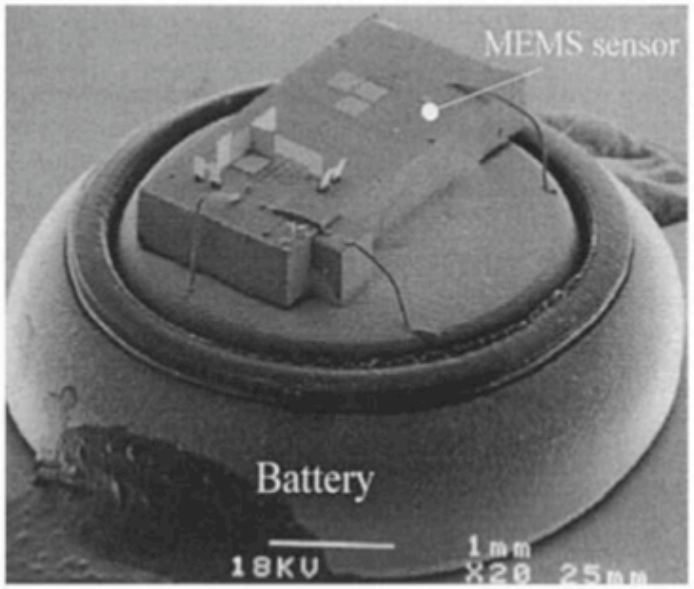


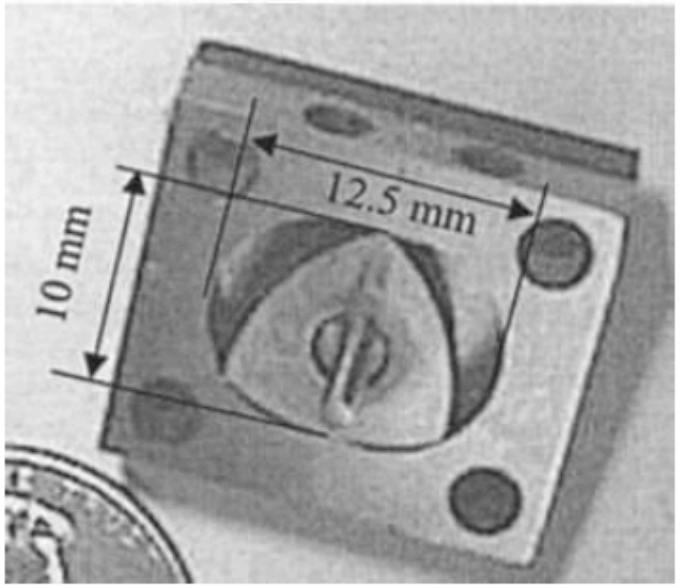
Electrically-induced extinction of
a $CH_4$ jet diffusion flame.
Credits: Prof. G.M. Whitesides (Harvard)

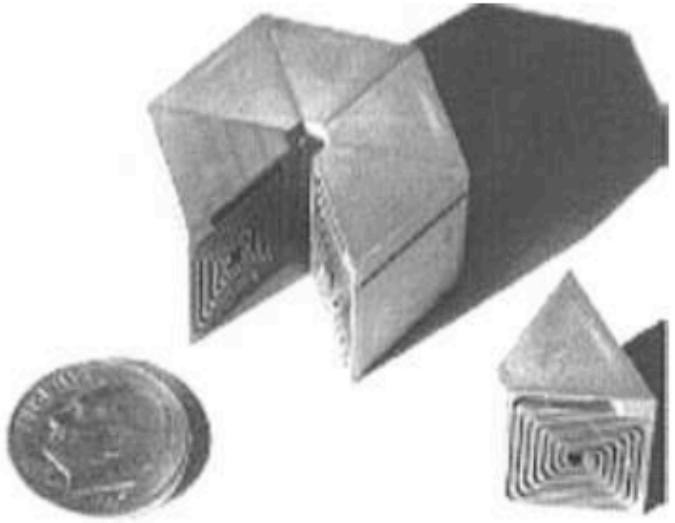
(Movie)

# Combustion in propulsion engineering

7. MICRO-PROPULSION/ENERGIZATION





Hydrogen-Bubble Propelled PANI/Zn Microrocket



Magnetic Control of Ni/Ti/PANI/Zn Microro



$H_2$-powered microrockets
Credits: Prof. J. Wang (UCSD)

(Movie)

STANFORD MECHANICAL ENGINEERING

**ME 471: TURBULENT COMBUSTION**

**Spring 2012**

# References

(by chronological order of appearance in class)

J. Urzay

Liñán (1974) ``Asymptotic structure of counterflow diffusion flames for large activation energies''

Williams (1985) ``Combustion theory”

Peters and Williams (1987) ``The asymptotic structure of stoichiometric methane-air flames''

Peters (1983) ``Local quenching due to flame stretch and non-premixed turbulent combustion''

Balakrishnan, Smooke and Williams (1995) ``A numerical investigation of extinction and ignition limits in laminar nonpremixed counterflowing hydrogen-air streams for both elementary and reduced chemistry''

Boivin, Jimenez, Sánchez and Williams (2011) ``An explicit reduced mechanism for H2-air combustion''

Kolmogorov (1941) ``The local structure of turbulence in incompressible viscous fluid for very large Reynolds numbers''

Broadwell and Mungal (1993) ``Large-scale structures and molecular mixing''

Jimenez (2004) ``Turbulence and vortex dynamics''

Pitsch (2006) ``Large-eddy simulation of turbulent combustion''

Liñán and Williams (1993) ``Fundamental aspects of combustion”

Echekki (2004) ``Multiscale methods in turbulent combustion: Strategies and computational challenges''

Poinsot and Veynante (2005) ``Theoretical and numerical combustion”

Matalon and Matkowsky (1982) ``Flames as gasdynamic discontinuities''

Clanet and Searby (1998) ``First experimental study of the Darrieus-Landau instability''

Clavin and Williams (1982) ``Effects of molecular diffusion and thermal expansion on the structure and dynamics of premixed flames in turbulent flows of large scale and low intensity''

Ronney, Wu, Pearlman and Weiland (1998) ``Experimental study of flame balls in space: Preliminary results from STS-83''

Spalding (1976) ``Mathematical models of turbulent flames''

Veynante and Vervisch (2002) ``Turbulent combustion modeling''

Libby and Bray (1981) ``Countergradient diffusion in premixed turbulent flames''

Bray, Libby and Moss (1984) ``Flamelet crossing frequencies and mean reaction rates in premixed turbulent combustion''

Haworth and Poinsot (1992) ``Numerical simulations of Lewis number effects in turbulent premixed flames''

Marble and Broadwell (1977) ``The coherent flame model for turbulent chemical reactions''

Vervisch, Bidaux, Bray and Kollmann (1994) ``Surface density function in premixed turbulent combustion modeling, similarities between probability density function and flame surface approaches''

Hawkes and Cant (2007) ``A flame surface density approach to large-eddy simulation of premixed turbulent combustion''

Peters (1992) ``A spectral closure for premixed turbulent combustion in the flamelet regime''

Peters (1999) ``The turbulent burning velocity for large-scale and small-scale turbulence''

Kerstein, Ashurst and Williams (1988) ``Field equation for interface propagation in an unsteady homogeneous flow field''

Peters (1988) ``Laminar flamelet concepts in turbulent combustion''

Joulin (1994) ``On the response of premixed flames to time-dependent stretch and curvature''

Pitsch and Duchamp de Lageneste (2002) ``Large-eddy simulation of premixed turbulent combustion using a level-set approach''

Liñán (1991) ``The structure of diffusion llames''

Liñán, Orlandi, Verzicco and Higuera (1994) ``Effects of non-unity Lewis numbers in diffusion flames''

Clavin and Liñán (1984) ``Theory of gaseous combustion''

Williams (2000) ``Progress in knowledge of flamelet structure and extinction''

Effelsberg and Peters (1983) ``A composite model for the conserved scalar pdf''

Luo and Bray (1998) ``Combustion-induced pressure effects in supersonic diffusion flames''

Pitsch and Peters (1998) ``A consistent flamelet formulation for non-premixed combustion considering differential diffusion effects''

Pierce and Moin (2004) ``Progress-variable approach for large-eddy simulation of non-premixed turbulent combustion''

# ME 471: TURBULENT COMBUSTION

## Spring 2012

**MAIN CONCEPTS**



STANFORD MECHANICAL ENGINEERING

**ME 471: TURBULENT COMBUSTION**

**Spring 2012**

# PART I:

# Fundamental Concepts in Combustion and Turbulent Flows

J. Urzay

# I. CONSERVATION EQUATIONS FOR REACTING FLOWS

J. URZAY

- CONTINUITY: $\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho \underline{v}) = 0$ (↳ CHEMICAL REACTIONS DO NOT GENERATE / DESTROY MASS) OR $\frac{D\rho}{Dt} = -\rho \nabla\cdot\underline{v}$ (↳ NET CHANGE OF VOLUME IN A FLUID PARTICLE) IF $\frac{D}{Dt} = \frac{\partial}{\partial t} + \underline{v}\cdot\nabla$ (1)

- MOMENTUM: $\rho\frac{\partial \underline{v}}{\partial t} + \rho\,\underline{v}\cdot\nabla\underline{v} = -\nabla P + \nabla\cdot\bar{\bar{\tau}}' + \sum_{i=1}^{N} \rho Y_i \underline{f}_i$ (2) WITH $N$ = NUMBER OF SPECIES, $Y_i = \rho_i/\rho$ MASS FRACTION OF SPECIES $i$

AND $\bar{\bar{\tau}}' = \mu(\nabla\underline{v} + \nabla\underline{v}^T) + \lambda\nabla\cdot\underline{v}$ FOR NEWTONIAN FLUIDS;

BULK VISCOSITY: NON-EQUILIBRIUM EFFECTS BECAUSE OF SUDDEN EXPANSIONS AND COMPRESSIONS (SHORT LIVED)

$\lambda = \left(k - \frac{2}{3}\right)\mu$ IS THE 2ND COEFFICIENT OF VISCOSITY. WITH $\lambda = -\frac{2}{3}\mu$ FOR MONOATOMIC GASES ($k=0$)

SINCE $\underline{v}\cdot\nabla\underline{v} = \nabla\left(\frac{|\underline{v}|^2}{2}\right) - \underline{v}\wedge\nabla\wedge\underline{v}$, THEN $\underline{v}\cdot(\underline{v}\cdot\nabla\underline{v}) = \frac{1}{2}\underline{v}\cdot\nabla\left(\frac{|\underline{v}|^2}{2}\right)$

PROOF: $(\nabla\wedge\underline{v})_i = \varepsilon_{ijk}\frac{\partial v_k}{\partial x_j}$

WITH $\varepsilon_{ijk}\varepsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$

$\Rightarrow (\underline{v}\wedge\nabla\wedge\underline{v})_i = \varepsilon_{ijk} v_j (\nabla\wedge\underline{v})_k =$

$= \varepsilon_{ijk} v_j \varepsilon_{klm}\frac{\partial v_m}{\partial x_l} =$

$= (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}) v_j \frac{\partial v_m}{\partial x_l} =$

$= v_j\frac{\partial v_j}{\partial x_i} - v_j\frac{\partial v_i}{\partial x_j} = \frac{\partial}{\partial x_i}\left(\frac{v_j v_j}{2}\right) - v_j\frac{\partial v_i}{\partial x_j}$

$\nabla\times\nabla\phi = 0$, $\nabla\cdot(\nabla\wedge\phi) = 0$

AND A KINETIC ENERGY EQUATION CAN BE OBTAINED BY MULTIPLYING (2) BY $\underline{v}$ IN SCALAR PRODUCT:

$$\rho\frac{\partial}{\partial t}\left(\frac{|\underline{v}|^2}{2}\right) + \rho\,\underline{v}\cdot\nabla\left(\frac{|\underline{v}|^2}{2}\right) = -\underline{v}\cdot\nabla P + \underline{v}\cdot\nabla\bar{\bar{\tau}}' + \sum_{i=1}^{N}\rho Y_i \underline{f}_i\cdot\underline{v} \quad (3)$$

NOTICE THAT, BECAUSE OF MASS CONSERVATION:

$$\rho\frac{\partial\phi}{\partial t} + \rho\,\underline{v}\cdot\nabla\phi = \frac{\partial}{\partial t}(\rho\phi) + \nabla\cdot(\rho\underline{v}\phi) - \phi\underbrace{\left(\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\underline{v})\right)}_{=0} = \frac{\partial}{\partial t}(\rho\phi) + \nabla\cdot(\rho\underline{v}\phi)$$

- TOTAL INTERNAL ENERGY:

$$e_t = e + \frac{|\underline{v}|^2}{2}, \text{ WITH } e = h - \frac{P}{\rho} = \sum_{i=1}^{N} Y_i h_i^0 + \sum_{i=1}^{N} Y_i\int_T^T c_{p_i}dT - \frac{P}{\rho}$$

WITH $h = \sum_{i=1}^{N} Y_i h_i = \underbrace{\sum_{i=1}^{N} Y_i h_i^0}_{\text{CHEMICAL ENTHALPY}} + \underbrace{\sum_{i=1}^{N} Y_i\int c_{p_i}dT}_{\text{SENSIBLE ENTHALPY}}$, $c_p = \underbrace{\sum_{i=1}^{N} Y_i c_{p_i}}_{\text{VARIES WITH } T,\ \text{SEE FIG 1.}}$

THEN $$\rho\frac{\partial e_t}{\partial t} + \rho\,\underline{v}\cdot\nabla e_t = -\nabla\cdot(P\underline{v}) + \nabla\cdot(\bar{\bar{\tau}}'\cdot\underline{v}) + \sum_{i=1}^{N}\rho Y_i\underline{f}_i\cdot(\underline{v} + \underline{V}_i) - \nabla\cdot\underline{q}'' + \dot{Q}_R \quad (4)$$

WHERE $\underline{V}_i$ IS THE DIFFUSION VELOCITY, $\dot{Q}_R$ IS THE RADIATION HEAT AND

$$\underline{q}'' = -\lambda\nabla T + \underbrace{\sum_{i=1}^{N}\rho h_i Y_i \underline{V}_i}_{\text{HEAT DIFFUSION BY NON-EQUAL ENTHALPIES}} + \underbrace{R^0 T\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{X_i D_{T,i}}{W_i D_{ij}}(\underline{V}_i - \underline{V}_j)}_{\text{HEAT DIFFUSION BY CONCENTRATION GRADIENTS : DUFOUR EFFECT}} \quad (5)$$

THE HEAT FLUX

BINARY DIFFUSION COEFFICIENT

FOR H ATOMS IN AIR $Y_H \sim \frac{X_H W_H}{\overline{W}} \ll X_H$

} RECIPROCAL CROSS-TRANSPORT VS SORET EFFECT, ONSAGER

HERE $X_i = \frac{N_i}{N_t} = \frac{Y_i/W_i}{\sum_{i=1}^{N} Y_i/W_i} = \frac{Y_i\overline{W}}{W_i}$ IS THE MOLAR FRACTION, $\overline{W}$ THE MEAN MOLECULAR WEIGHT

AND $D_{T,i}$ IS A THERMAL-DIFFUSION COEFFICIENT, WHICH MAY BE > OR < 0 DEPENDING ON PRESSURE, TEMPERATURE AND CONCENTRATIONS, AND WHICH IS NEGLIGIBLE $\left(\frac{D_{T,i}}{\rho D_{ij}} < \frac{1}{10}\right)$ IN ALMOST ALL SITUATIONS.
⇒ SHOULD NOT BE CONFUSED WITH THE THERMAL DIFFUSIVITY $D_T = \frac{\lambda}{\rho c_p}$.

- TOTAL ENTHALPY: $h_t = h + \frac{|\underline{v}|^2}{2}$, WITH $h = \sum_{i=1}^{N} h_i Y_i \simeq e + \frac{P}{\rho}$

THEN $\frac{Dh_t}{Dt} = \frac{De_t}{Dt} + \frac{1}{\rho}\frac{DP}{Dt} - \frac{P}{\rho^2}\frac{D\rho}{Dt} = \frac{De_t}{Dt} + \frac{1}{\rho}\frac{DP}{Dt} + \frac{P}{\rho}\nabla\cdot\underline{v} = \frac{De_t}{Dt} + \frac{1}{\rho}\left(\frac{\partial P}{\partial t} + P\nabla\cdot\underline{v} + \underline{v}\cdot\nabla P\right)$

AND $$\rho\frac{\partial h_t}{\partial t} + \rho\,\underline{v}\cdot\nabla h_t = \frac{\partial P}{\partial t} + \nabla\cdot(\bar{\bar{\tau}}'\cdot\underline{v}) - \nabla\cdot\underline{q}'' + \sum_{i=1}^{N}\rho Y_i\underline{f}_i(\underline{V}_i + \underline{v}) + \dot{Q}_R \quad (6)$$

- STATIC ENTHALPY: $h = h_t - \frac{|\underline{v}|^2}{2}$. SUBSTRACTING (8) FROM (6) THE EQUATION

$$\rho\frac{\partial h}{\partial t} + \rho\,\underline{v}\cdot\nabla h = \frac{DP}{Dt} + \bar{\bar{\tau}}':\nabla\underline{v} - \nabla\cdot\underline{q}'' + \sum_{i=1}^{N}\rho Y_i\underline{f}_i\cdot\underline{V}_i + \dot{Q}_R \quad (7)$$

SINCE $\nabla\cdot(\bar{\bar{\tau}}'\cdot\underline{v}) = \underline{v}\cdot\nabla\cdot\bar{\bar{\tau}}' + \bar{\bar{\tau}}':\nabla\underline{v}$

$\Rightarrow \frac{\partial}{\partial x_j}(\tau_{ij}v_i) = v_i\frac{\partial\tau_{ij}}{\partial x_j} + \tau_{ij}\frac{\partial v_i}{\partial x_j}$

- INTERNAL ENERGY: $e = h - \frac{P}{\rho}$ →

$$\rho\frac{\partial e}{\partial t} + \rho\,\underline{v}\cdot\nabla e = -P\nabla\cdot\underline{v} + \bar{\bar{\tau}}':\nabla\underline{v} - \nabla\cdot\underline{q}'' + \sum_{i=1}^{N}\rho Y_i\underline{f}_i\cdot\underline{V}_i + \dot{Q}_R \quad (8)$$

- SPECIES: $Y_i = \frac{\rho_i}{\rho} = \frac{X_i W_i}{\sum_{i=1}^{N} X_i W_i} = \frac{m_i}{m\rho} = \frac{N_i W_i}{m\rho} = \frac{[\bar{n}_i] W_i}{\rho}$ , $[i]$ = MOLAR CONCENTRATION

$\Rightarrow \frac{\partial \rho_i}{\partial t} + \nabla\cdot(\rho_i \underline{v}_i) = \dot{W}_i$ = RATE OF PRODUCTION OF SPECIES "$i$" $\left[\frac{kg}{m^3 s}\right]$ $\rightarrow \sum_{i=1}^{N} \dot{W}_i = 0$

AND $\underline{V}_i$ = VELOCITY OF SPECIES "$i$" $= \underline{v} + \underline{V_i}$ — DIFFUSION VELOCITY

$\sum_{i=1}^{N} Y_i \underline{V}_i = 0$

THEN $\boxed{\rho \frac{\partial Y_i}{\partial t} + \rho \underline{v}\cdot\nabla Y_i = -\nabla\cdot(\rho \underline{V}_i Y_i) + \dot{W}_i}$ (9) → SEE SCALING PAGE

↳ CENTRAL TO COMBUSTION SCIENCE: ACCUMULATION + ADVECTION BY MASS-AVERAGE MOTION OF THE FLUID + DIFFUSION + PRODUCTION

IN TERMS OF CONCENTRATIONS: $\Gamma_i = \frac{c_i}{\rho} = \frac{Y_i}{W_i} \Rightarrow \rho \frac{\partial \Gamma_i}{\partial t} + \rho \underline{v}\cdot\nabla \Gamma_i = -\nabla\cdot(\rho \underline{V}_i \Gamma_i) + \frac{\dot{W}_i}{W_i}$ ($\frac{mol}{m^3 s}$)

- NON-CHEMICAL INTERNAL ENERGY: $e_s = e - \sum_{i=1}^{N} Y_i h_i^\circ \rightarrow \frac{De_s}{Dt} = \frac{De}{Dt} - \sum_{i=1}^{N} h_i^\circ \frac{DY_i}{Dt}$

$\Rightarrow \boxed{\frac{\partial e_s}{\partial t} + \rho \underline{v}\cdot\nabla e_s = -P\nabla\cdot\underline{v} + \bar{\bar{\tau}}' : \nabla\underline{v} + \nabla\cdot\left(\kappa\nabla T - \sum_{i=1}^{N} \rho h_{s_i} Y_i \underline{V}_i\right) + \sum_{i=1}^{N} \rho Y_i \underline{f}_i\cdot\underline{V}_i - \sum_{i=1}^{N} \dot{W}_i h_i^\circ + \dot{Q}_R}$

WITH $h_{s_i} = \int^T c_{p_i} dT$ → 0 WHEN $c_{p_i} = c_p$ (10)

- NON-CHEMICAL ENTHALPY: $h_s = h - \sum_{i=1}^{N} Y_i h_i^\circ = e_s + \frac{P}{\rho}$

$\Rightarrow \boxed{\rho \frac{\partial h_s}{\partial t} + \rho \underline{v}\cdot\nabla h_s = \frac{DP}{Dt} + \bar{\bar{\tau}}' : \nabla\underline{v} + \nabla\cdot\left(\kappa\nabla T - \sum_{i=1}^{N} \rho h_{s_i} Y_i \underline{V}_i\right) + \sum_{i=1}^{N} \rho Y_i \underline{f}_i\cdot\underline{V}_i - \sum_{i=1}^{N} \dot{W}_i h_i^\circ + \dot{Q}_R}$ (11)

AN ALTERNATIVE EXPRESSION CAN BE OBTAINED BY MAKING $\frac{Dh_s}{Dt} = \frac{D}{Dt}\sum_{i=1}^{N} Y_i \int^T c_{p_i} dT = \sum_{i=1}^{N} \frac{DY_i}{Dt}\int^T c_{p_i} dT + \sum_{i=1}^{N} \rho Y_i c_{p_i} \frac{DT}{Dt} = \sum_{i=1}^{N} \dot{W}_i \int^T c_{p_i} dT - \sum_{i=1}^{N} \nabla\cdot(\rho \underline{V}_i Y_i)\cdot \int^T c_{p_i} dT + \sum_{i=1}^{N} c_p \frac{DT}{Dt}$

WITH $c_p = \sum_{i=1}^{N} Y_i c_{p_i} = c_v + R^\circ/\overline{W}$ THE MEAN SPECIFIC HEAT.

THEN (11) BECOMES $\boxed{\rho c_p \frac{\partial T}{\partial t} + \rho c_p \underline{v}\cdot\nabla T = \frac{DP}{Dt} + \bar{\bar{\tau}} : \nabla\underline{v} + \nabla\cdot(\kappa\nabla T) - \sum_{i=1}^{N} \rho \underline{V}_i Y_i c_{p_i}\nabla T + \sum_{i=1}^{N} \rho Y_i \underline{f}_i\cdot\underline{V}_i + \dot{Q}_R - \sum_{i=1}^{N} h_i \dot{W}_i}$ (12)

$\bar{\bar{\tau}}' : \nabla\underline{v} \sim O(M^2/Re)$

- IDEAL GAS: $\boxed{P = \rho \frac{R^\circ T}{\overline{W}}}$ HOLDS AND $c_p - c_v = \frac{R}{\overline{W}}$ (CAN HAVE VIBRATIONAL / ROTATIONAL DEGREES OF FREEDOM, AS LONG AS THEY ARE DECOUPLED)

↳ IF THIS HAPPENS $e$ / MAY HAVE A COMPLEX FORM WITH $T$

- CALORICALLY-PERFECT GAS: IDEAL + $c_p, c_v \neq f(T)$

- VORTICITY EQUATION: OBTAINED BY TAKING $\nabla \wedge (2)$:

$\boxed{\frac{\partial \underline{\omega}}{\partial t} + \underline{v}\cdot\nabla\underline{\omega} = \underline{\omega}\cdot\nabla\underline{v} - \underline{\omega}\nabla\cdot\underline{v} + \frac{1}{\rho^2}\nabla\rho\wedge\nabla P + \nabla\wedge\left(\frac{\nabla\cdot\bar{\bar{\tau}}}{\rho}\right) + \sum_{i=1}^{N} \nabla\wedge(\underline{f}_i Y_i)}$ (13)

VORTEX STRETCH — COMPRESSIBILITY — BAROCLINIC TORQUE — VISCOUS GENERATION OF $\underline{\omega}$ — $\neq 0$ FOR NON-CONSERVATIVE FORCES.

BAROCLINIC TORQUE: RESPONSIBLE FOR VORTICITY GENERATION BEHIND CURVED FLAMES

IN TURBULENT COMBUSTION $\frac{T_b}{T_u} \sim 8$, $D \sim T^{0.7} \rightarrow \frac{D_b}{D_u} \sim 40$, $\rightarrow Re_u \sim 40 Re_b$ ↳ VORTICITY IS ATTENUATED

- MOLECULAR DIFFUSION: THE DIFFUSION VELOCITIES ARE OBTAINED FROM

$\boxed{\nabla X_i = \sum_{j=1}^{N}\left(\frac{X_i X_j}{D_{ij}}\right)(\underline{V}_j - \underline{V}_i) + (Y_i - X_i)\left(\frac{\nabla P}{P}\right) + \left(\frac{\rho}{P}\right)\sum_{j=1}^{N} Y_i Y_j (\underline{f}_i - \underline{f}_j) + \sum_{j=1}^{N}\left[\left(\frac{X_i X_j}{\rho D_{ij}}\right)\left(\frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i}\right)\right]\left(\frac{\nabla T}{T}\right)}$ (14)

CONCENTRATION GRADIENTS — BARODIFFUSION — THERMAL DIFFUSION (SORET)

DELAYS EXTINCTION AND ENHANCES PROPAGATION IN $H_2$ FLAMES → SEE FIG. 2

COSTLY ($N^2$ LINEAR SYSTEM IN $\underline{V}$) — ONSAGER RECIPROCAL TREATMENT

TENDS TO PUSH LIGHT MOLECULES ($H_2$) TO HOT REGIONS AND HEAVY MOLECULES (SOOT, $N_2$) TO COLD REGIONS

FOR SYSTEMS IN WHICH: i) THERMAL DIFFUSION IS NEGLIGIBLE

ii) THE BODY FORCE PER UNIT MASS IS THE SAME IN EACH SPECIES

iii) THE PRESSURE GRADIENTS ARE SMALL OR THE MOLECULAR WEIGHTS ARE THE SAME

THEN $$\nabla X_i = \sum_{j=1}^{N} \frac{X_i X_j}{D_{ij}} \left( \underline{V}_j - \underline{V}_i \right)$$ STEFAN-MAXWELL EQUATION (15)

IF, ADDITIONALLY, THE MIXTURE IS BINARY: $Y_1 + Y_2 = 1$ AND $Y_1 \underline{V}_1 + Y_2 \underline{V}_2 = 0$

AND (15) REDUCES TO $$\underline{Y_1 V_1} = - D_{12} \nabla Y_1$$ (16) ⇒ FICKIAN DIFFUSION

PROOF: $X_1 = \frac{Y_1 \bar{W}}{W_1}$, $X_2 = \frac{Y_2 \bar{W}}{W_2}$

$\Rightarrow \nabla X_1 = \frac{\bar{W}}{W_1} \nabla Y_1 + Y_1 \frac{\nabla \bar{W}}{W_1}$

$\Rightarrow \frac{Y_1 Y_2}{D_{12}} \left( \underline{V}_2 - \underline{V}_1 \right) \frac{\bar{W}^2}{W_1 W_2} = \frac{\bar{W}}{W_2} \nabla Y_1 + \frac{Y_1}{W_1} \nabla \bar{W}$

SINCE $\underline{V}_2 = -\frac{\underline{V}_1 Y_1}{Y_2}$ AND $Y_2 = 1 - Y_2$

THEN $- \frac{\underline{V}_1 Y_1}{D_{12}} = \left( \frac{Y_1 W_2}{W_1} + (1 - Y_1) \right) \nabla Y_1 - Y_1 W_2 \nabla \left( \frac{1}{\bar{W}} \right) =$

$= \frac{Y_1 W_2}{W_1} \nabla Y_1 + \nabla Y_1 - Y_1 \nabla Y_1 - \frac{Y_1 W_2}{W_1} \nabla Y + Y_1 \nabla$

IN MULTISPECIES SYSTEMS, USE IS OFTEN MADE OF THE "HIRSCHFELDER AND CURTISS APPROXIMATION", WHICH IS A LEADING-ORDER SOLUTION OF THE STEFAN-MAXWELL EQUATION: ⇝ PSEUDO-BINARY LIMIT ($Y_i + Y_N = 1$, $Y_i \ll Y_N$)

$$\underline{V_i} X_i = - D_i \nabla X_i$$ (17) WITH $D_i = \frac{1 - Y_i}{\sum_{j \neq i}^{N} X_j / D_{ij}}$ AN EQUIVALENT

$\frac{\underline{V_i}}{W_i} = \frac{W_i}{\bar{W}}$ DIFFUSION COEFFICIENT OF SPECIES "i" INTO THE MIXTURE. → STILL NEEDED

SO THAT (9) BECOMES $\rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla Y_i = - \nabla \cdot \left( \rho D_i \frac{W_i}{\bar{W}} \nabla X_i \right) + \dot{w}_i$

HOWEVER, $\sum_{i=1}^{N} \rho D_i \frac{W_i}{\bar{W}} \nabla X_i \neq 0$ SO THAT IN GENERAL, A CORRECTION VELOCITY $\underline{V_c}$ NEEDS TO BE TO THE CONVECTION VELOCITY TO ENSURE THE COMPATIBILITY BETWEEN SPECIES AND MASS CONSERVATION. IN PARTICULAR, $\underline{V_c}$ IS SUCH THAT $\sum_{i=1}^{N} \underline{V_i} Y_i + \underline{V_c} = 0$, WITH $\underline{V_i}$ GIVEN BY (17), SO THAT $$\underline{V_c} = \sum_{i=1}^{N} D_i \frac{W_i}{\bar{W}} \nabla X_i$$, SO THAT (9) SHOULD READ $\rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla Y_i = + \nabla \cdot \left[ \rho D_i \frac{W_i}{\bar{W}} \nabla X_i - \sum_{i=1}^{N} \rho D_i \frac{W_i}{\bar{W}} \nabla X_i \right] + \dot{w}_i$

IF USE IS NOT MADE OF THE CORRECTION VELOCITY, THEN THE DILUENT MASS FRACTION IS OBTAINED BY WRITING $Y_{N_2} = 1 - \sum_{i \neq N_2}^{N} Y_i$, THUS ABSORBING THE INCONSISTENCY INTRODUCED BY (17). IF $\underline{V_c}$ IS USED, THEN THE SOLUTION OF THE DILUENT TRANSPORT EQUATION IS CONSISTENT WITH THE OTHER MASS-FRACTION DISTRIBUTIONS AND WITH MASS CONSERVATION. (17) IS EXACT FOR BINARY MIXTURES AND REDUCES TO (16).

- DIMENSIONLESS PARAMETERS RELATED TO DIFFUSION:

# LEWIS: $Le_i = \frac{D_T}{D_i} = \frac{k}{\rho c_p D_i}$;

# PRANDTL: $Pr = \frac{\nu}{D_T} = \frac{\mu / \rho}{k / \rho c_p} = \frac{\mu c_p}{k}$

# SCHMIDT: $Sc_i = \frac{\nu}{D_i} = \frac{\mu}{\rho D_i}$

SINCE $k \sim T^{\sigma}$, $\sigma = 0.7$, $\mu \sim T^{\sigma}$, $\rho \sim 1/T$, $D_i \sim T^{1+\sigma}$;

THEN $Sc_i$, $Pr$ AND $Le_i$ VARY LITTLE WITH $T$ (MAINLY DUE TO T-VARIATIONS OF $c_p$) → SEE FIG 1.

- LOW-MACH LIMIT: AT LOW MACH NUMBERS, THE TIMESTEP REQUIRED IN EXPLICIT DISCRETIZATIONS IS OF ORDER $\Delta t \sim \Delta x / c$ IN ORDER TO FOLLOW THE SOUNDWAVES. HOWEVER, THE ENERGY CARRIED BY THE SOUNDWAVES IN LOW-MACH FLOWS IS TYPICALLY NOT IMPORTANT




TAKING DIMENSIONLESS VARIABLES $\underline{V}^* = \underline{V}/v_0$, $P^* = P/P_0$, $\rho^* = \rho/\rho_0$, $T^* = T/T_0$, $x^* = x/L$, $t^* = t/t_0$

⇒ $\Delta t_{phys} = \frac{\Delta x}{v} = \frac{\Delta t}{M}$ THE DIMENSIONLESS CONTINUITY, MOMENTUM, AND EQ OF STATE BECOME:

$P^* = \rho^* R^* T^*$, $\frac{\partial \rho^*}{\partial t^*} + \nabla \cdot (\rho^* \underline{v}^*) = 0$, $\rho^* \frac{\partial \underline{v}^*}{\partial t^*} + \rho^* \underline{v}^* \cdot \nabla \underline{v}^* = - \frac{\nabla P^*}{M^2} + \frac{1}{Re} \nabla \cdot \bar{\tau}^*$

AT LOW MACH NUMBERS $M = v/c \ll 1$, THE DEPARTURES OF THE PRESSURE FROM ITS BACKGROUND VALUE $P_0$ ARE GENERATED BY DYNAMIC-PRESSURE VARIATIONS AND THEY ARE SMALL ($\mathcal{O}(M^2)$). A SERIES-EXPANSION FOR THE PRESSURE YIELDS: $P^* = P_0^* + M^2 \Pi$

$P_0^* = \rho^* R^* T^*$ → $\nabla P_0 = 0$ → $P_0 = P_0(t)$

$\frac{\partial \rho^*}{\partial t^*} + \nabla \cdot (\rho^* \underline{v}^*) = 0$ AND $\rho^* \frac{\partial \underline{v}^*}{\partial t^*} + \rho^* \underline{v}^* \cdot \nabla \underline{v}^* = - \nabla \Pi + \frac{1}{Re} \nabla \cdot \bar{\tau}'$

↳ A POISSON EQUATION CAN BE CONSTRUC

THEN THE PROCEDURE IS TO SOLVE DENSITY FROM TEMPERATURE FIELD, SOLVE MOMENTUM FOR A GIVEN $\Pi$, SOLVE A POISSON EQUATION FOR $\Pi$, AND ITERATE.

- SIMPLIFIED FORMS: → LOW MACH:

$$\begin{cases} p_0 = \rho \frac{R}{\bar{W}} T \\ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = 0 \\ \rho \frac{\partial \underline{v}}{\partial t} + \rho \underline{v} \cdot \nabla \underline{v} = -\nabla \Pi + \nabla \cdot \bar{\bar{\tau}}' + \sum_{i=1}^{N} \rho Y_i \underline{f}_i \\ \rho c_p \frac{\partial T}{\partial t} + \rho c_p \underline{v} \cdot \nabla T = \frac{D p_0}{D t} + \nabla \cdot (\kappa \nabla T) - \sum_{i=1}^{N} \rho \underline{V}_i Y_i c_{pi} \nabla T \\ \qquad + \sum_{i=1}^{N} \rho Y_i \underline{f}_i \cdot \underline{V}_i + \dot{Q}_R - \sum_{i=1}^{N} h_i \dot{w}_i \\ \rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla Y_i = -\nabla \cdot (\rho \underline{V}_i Y_i) + \dot{w}_i \end{cases}$$

+ EQUAL HEAT CAPACITIES: $c_p = c_{pi}$:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p \underline{v} \cdot \nabla T = \frac{D p_0}{D t} + \nabla \cdot (\kappa \nabla T) + \sum_{i=1}^{N} \rho Y_i \underline{f}_i \cdot \underline{V}_i + \dot{Q}_R - \sum_{i=1}^{N} h_i^{\circ} \dot{w}_i$$

+ FICKIAN DIFFUSION:

$$\rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla Y_i = + \nabla \cdot (\rho D_i \nabla Y_i) + \dot{w}_i$$

- COUPLING FUNCTIONS:

$$\begin{cases} \rho \frac{\partial T}{\partial t} + \rho \underline{v} \cdot \nabla T = \nabla \cdot \left( \frac{\kappa}{c_p} \nabla T \right) + q \frac{\dot{w}_R}{c_p} \\ \rho \frac{\partial Y_R}{\partial t} + \rho \underline{v} \cdot \nabla Y_R = \nabla \cdot (\rho D_R \nabla Y_R) - \dot{w}_R \end{cases}$$

$R \rightarrow P + q$ (q: CHEMICAL HEAT RELEASED)

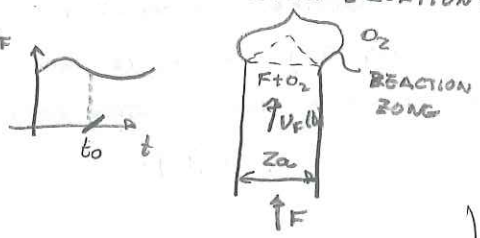
FOR $Le = \frac{k}{\rho c_p D_R} = 1$, THESE TWO EQUATIONS CAN BE COMBINED TO GIVE

$$\rho \frac{\partial H}{\partial t} + \rho \underline{v} \cdot \nabla H = \nabla \cdot (\rho D \nabla H), \quad \text{WITH } H = c_p T + \frac{Y_F q}{R T}$$

THE EXCESS ENTHALPY

⇒ SHVAB - ZEL'DOVICH FORMULATION OF COUPLING FUNCTIONS.

- THE SPECIES TRANSPORT EQUATION:




$$\underbrace{\frac{\partial Y_F}{\partial t}}_{O\left(\frac{1}{t_0}\right)} + \underbrace{\underline{v} \cdot \nabla Y_F}_{O\left(\frac{U_F}{a}\right) \to 1/t_r} = \underbrace{-\frac{1}{\rho} \nabla \cdot (\rho Y_F \underline{V}_F)}_{O\left(\frac{D_F}{a^2}\right) \to t_d} + \underbrace{\frac{\dot{w}_F}{\rho}}_{O\left(\frac{1}{t_{exc}}\right)}$$

ACCUMULATION — ADVECTION — DIFFUSION — CHEMICAL REACTION

$t_c$ = CHEMICAL TIME; $t_r$ = RESIDENCE TIME; $t_d$ = DIFFUSION TIME

$$\begin{cases} \#\ \text{STROUHAL} = St = \frac{a/U_F}{t_0} = \frac{t_r}{t_0} \\ \#\ \text{PECLET}: \ Pe = \frac{t_d}{t_r} = \frac{U_F a}{D_F} = \frac{U_F a}{\mathcal{D}} \frac{\mathcal{D}}{D_F} = Re \cdot Sc \\ \#\ \text{DAMKÖHLER}: \ Da = \frac{t_r}{t_{coll}} = \frac{a}{U_F t_{coll}} \quad (\text{COLLISION}) \end{cases}$$

## D3 : CHEMICAL REACTION RATES

- GIVEN A MECHANISM $\sum_{i=1}^{N} \nu_{ij}' \mathcal{R}_i \rightleftharpoons \sum_{i=1}^{N} \nu_{ij}'' \mathcal{R}_i$ WITH N SPECIES AND M ELEMENTARY STEPS, THE NET REACTION RATE (LAW OF MASS ACTION (PHENOMENOLOGICAL))

$$\dot{\omega}_i = \frac{d[\mathcal{R}_i]/dt}{(\nu_i'' - \nu_i')} = k_{fj} \prod_{i=1}^{N} [\mathcal{R}_i]^{\nu_{ij}'} - k_{bj} \prod_{i=1}^{N} [\mathcal{R}_i]^{\nu_{ij}''} \quad \text{IN} \quad \left[ \frac{\text{mol}}{VT} \right] \quad (1)$$

→ REACTION RATE IS PROPORTIONAL TO THE COLLISION RATE BETWEEN MOLECULES, AND THE COLLISION RATE IS PROPORTIONAL TO THE PRODUCT OF THE CONCENTRATIONS

EQUATION (1) IS ONLY MEANINGFUL FOR:
- i) ELEMENTARY REACTION STEPS (i.e. PROCESSES THAT ACTUALLY OCCUR AT THE MOLECULAR LEVEL)
- ii) IS NOT MEANINGFUL FOR OVERALL STEPS ($CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ OR $2H_2 + O_2 \rightarrow 2H_2O$)

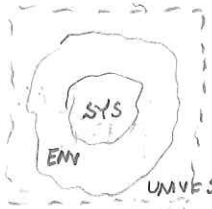
⇒ THE TWO MAIN PROBLEMS IN CHEMICAL KINETICS ARE:
- i) TO FIND THE SET OF ELEMENTARY REACTION RATES
- ii) TO DETERMINE THE SPECIFIC RATE CONSTANTS.

REACTION MOLECULARITY: $\sum_{i=1}^{N} \nu_i'$ (FORWARD), $\sum_{i=1}^{N} \nu_i''$ (BACKWARD) NUMBER OF MOLECULES THAT INTERACT IN THE PROCESS

IN CHEMICAL EQUILIBRIUM, $\dot{\omega}_j = 0$, AND $\frac{k_{fj}}{k_{bj}} = \prod_{i=1}^{N} [i]^{\nu_{ij}'' - \nu_{ij}'} = k_{cj}$, WITH $k_{cj}$ THE EQUILIBRIUM CONSTANT GIVEN BY $k_{cj} = \left(\frac{p^0}{R^0 T}\right)^{\sum_{i=1}^{N} \nu_{ij}'' - \nu_{ij}'} e^{-\sum_{i=1}^{N} \frac{(\nu_{ij}'' - \nu_{ij}') g_i^0}{R^0 T}}$, WITH $g_i^0(T)$ THE GIBBS FREE ENERGY OF SPECIES $i$ IN $J/mol$.

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* CHEMICAL EQUILIBRIUM: CONSIDER AN OPPOSING REACTION $\sum_{i=1}^{N} \nu_{ik}' \rightleftharpoons \sum_{i=1}^{N} \nu_{ij}''$. THE ZEROTH LAW OF THERMODYNAMICS STATES THAT THERE EXISTS AN ADDITIONAL INTENSIVE VARIABLE, TEMPERATURE $T$, WHICH HAS THE SAME VALUE FOR ALL SYSTEMS IN THERMODYNAMIC EQUILIBRIUM WITH EACH OTHER. THE FIRST LAW OF THERMODYNAMICS IS CONSERVATION OF ENERGY, WHICH STATES THAT THERE EXISTS AN EXTENSIVE FUNCTION $E = E(P, V, N_i)$, THE INTERNAL ENERGY, SUCH THAT $\delta Q = dE + P dV$, FOR A CLOSED SYSTEM, WITH $Q$ THE HEAT ADDED TO THE SYSTEM IN AN INFINITESIMAL PROCESS. MOREOVER, THE SECOND LAW OF THERMODYNAMICS ASSERTS THE EXISTENCE OF AN ABSOLUTE SCALE OF TEMPERATURE $T$ AND AN EXTENSIVE FUNCTION CALLED ENTROPY OF THE SYSTEM $S_{SYS}$ SUCH THAT $T dS_{SYS} \geq \delta Q$, WITH THE $=$ SIGN HOLDING ONLY FOR REVERSIBLE PROCESSES




A REVERSIBLE PROCESS IS A PROCESS PERFORMED IN SUCH A WAY THAT THE SYSTEM AND ITS SURROUNDINGS CAN BOTH RETURN TO THEIR INITIAL STATES → SLOW

IN GENERAL, $dS_{UNIV} = dS_{SYS} + dS_{ENV} \geq 0$, WITH $dS_{ENV} = -\frac{\delta Q}{T}$

- $dS_{UNIV}$: CHANGE OF ENTROPY IN UNIVERSE
- $dS_{SYS}$: CHANGE OF ENTROPY IN THE SYSTEM
- $dS_{ENV}$: CHANGE OF ENTROPY IN THE ENVIRONMENT
- $\delta Q$: HEAT

THE IRREVERSIBILITY IN CHEMICAL SYSTEMS IS RELATED TO THE IMBALANCE OF CHEMICAL POTENTIALS $\mu_i$ BETWEEN REACTANTS AND PRODUCTS, $T dS_{SYS} = \delta Q + \sum_{i=1}^{N} \mu_i dN_i$; SINCE THE GIBBS FREE ENERGY IS $G = H - TS = E + PV - TS$, THEN

AT $P = CONST$, $T = CONST$: $dG = -T dS_{UNIV} = +\sum_{i=1}^{N} \mu_i dN_i \leq 0$ ⇒ THE GIBBS FREE ENERGY OF THE CHEMICAL SYSTEM DECREASES AND REACHES REVERSIBILITY (CHEMICAL EQUILIBRIUM) WHEN $dG = 0$.

SINCE, FOR ANY TWO SPECIES $i$ AND $j$: $\frac{dN_i}{\nu_i'' - \nu_i'} = \frac{dN_j}{\nu_j'' - \nu_j'} = d\xi = \dot{\omega}_j dt =$ REACTION PROGRESS VARIABLE,

THEN $dG = \sum_{i=1}^{N} \mu_i (\nu_i'' - \nu_i') d\xi \leq 0$, OR EQUIVALENTLY, THE REACTION GOES IN THE FORWARD DIRECTION ($d\xi > 0$) WHEN THE CHEMICAL POTENTIAL DECREASES IN THE FORWARD DIRECTION, $\sum_{i=1}^{N} \mu_i (\nu_i'' - \nu_i') < 0$, AND REACHES CHEMICAL EQUILIBRIUM WHEN $\Delta G = 0 \leftrightarrow \sum_{i=1}^{N} \mu_i (\nu_i'' - \nu_i') = 0$

THE CHEMICAL-EQUILIBRIUM CONSTRAINT CAN BE WRITTEN AS: (FOR IDEAL GASES)

$$\sum_{i=1}^{N} \mu_i dN_i = \sum_{i=1}^{N} \left[ g_i^0(T) + R^0 T \ln\left(P_i / P^0\right) \right] dN_i = 0, \text{ OR, EQUIVALENTLY:}$$

$$-\sum_{i=1}^{N} \frac{(\nu_i'' - \nu_i') g_i^0(T)}{R^0 T} = \ln\left[ \prod_{i=1}^{N} \left( \frac{P_i}{P_0} \right)^{(\nu_i'' - \nu_i')} \right], \text{ AND SINCE } \frac{P_i}{P^0} = \frac{P_i}{P} \frac{P}{P^0} = X_i \frac{P}{P_0}$$

THEN

$$K_p = e^{-\sum_{i=1}^{N} \frac{(\nu_i'' - \nu_i') g_i^0(T)}{R^0 T}} = \prod_{i=1}^{N} X_i^{(\nu_i'' - \nu_i')} \left(\frac{P}{P_0}\right)^{(\nu_i'' - \nu_i')} = \prod_{i=1}^{N} [i]^{(\nu_i'' - \nu_i')} \left(\frac{RT}{P^0}\right)^{\nu_i'' - \nu_i'}$$

$$= \left(\frac{RT}{P^0}\right)^{\sum_{i=1}^{N} \nu_i'' - \nu_i'} \prod_{i=1}^{N} [i]^{(\nu_i'' - \nu_i')} = K_c \left(\frac{RT}{P^0}\right)^{\sum_{i=1}^{N} \nu_i'' - \nu_i'}$$

IS THE PRESSURE EQUILIBRIUM CONSTANT

---

THE TOTAL MASS OF SPECIES "$i$" PRODUCED PER UNIT VOLUME AND TIME IS $\dot{W}_i = W_i \sum_{j=1}^{M} (\nu_{ij}'' - \nu_{ij}') \dot{\omega}_j$

WITH $\sum_{i=1}^{N} \dot{W}_i = 0$ FOR MASS CONSERVATION.

THE CHEMICAL HEAT RELEASED PER UNIT VOLUME AND UNIT TIME IN EQ(12) IS

$$\dot{w}_T = -\sum_{i=1}^{N} h_{is} \dot{w}_i = -\sum_{i=1}^{N} \left( h_i^0 + \int^T c_{pi} dT \right) \dot{w}_i = -\sum_{i=1}^{N} \sum_{j=1}^{M} h_{is} W_i (\nu_{ij}'' - \nu_{ij}') \dot{\omega}_j = -\sum_{j=1}^{M} Q_j \dot{\omega}_j$$

WITH $Q_j = \sum_{i=1}^{N} W_i (\nu_i'' - \nu_i') h_{is}$ THE HEAT RELEASED IN $J/mol$ IN STEP $j$.

- THE RATE CONSTANT $k_i$, EITHER $k_i = k_f$ OR $k_i = k_b$, IS USUALLY WRITTEN IN THE ARRHENIUS APPROXIMATION: $\boxed{k_j = A_j T^{n_j} e^{-\frac{E_{aj}}{RT}}}$, WHICH ASSUMES THERMODINAMIC EQUILIBRIUM. THIS EQUATION STATES THAT THE REACTION RATE IS PROPORTIONAL TO THE PROBABILITY OF FINDING MOLECULES WITH KINETIC ENERGY HIGHER THAN THE ACTIVATION ENERGY.

$A_j$ = PRE-EXPONENTIAL FACTOR
$n_j$ = TEMPERATURE EXPONENT
$E_{aj}$ = ACTIVATION ENERGY

-NOTE THAT, FOR A UNIMOLECULAR REACTION: $\nu_1' \mathcal{R}_1 \rightarrow \nu_2'' \mathcal{R}_2$,

$\dot{\omega} = k [\mathcal{R}_1]^{\nu_1'}$, SO THAT $[k] = \left(\frac{MOL}{V}\right)^{1-\nu_1'} \frac{1}{T}$, AND

$k = A T^{\alpha} e^{\frac{-E_a}{RT}}$, WITH $[A] = \left(\frac{MOL}{V}\right)^{1-\nu_1'} \frac{1}{\text{TIME UNIT}} \frac{1}{\text{KELVINS}^{\alpha}}$ :

$\frac{d[\mathcal{R}_1]}{dt} = \dot{\omega}$

- A COLLISION CHEMICAL TIME CAN BE DEFINED AS $t_{COLL} \sim \left(k [\mathcal{R}_1]_0^{\nu_1'-1}\right)^{-1}$

- A LOCAL CHEMICAL TIME CAN BE DEFINED AS $t_c = \ln t_{COLL} \frac{[\mathcal{R}_1]_0^{\nu_1'-1}}{T_0^{\alpha}} e^{+\frac{E_a}{RT}}$

NOTE THAT $\uparrow T$ INVOLVES $\downarrow t_c$

⇒ INTEGRATIONS OF THE CONSERVATION EQUATIONS WITH $\dot{w}_k$ OR $\dot{w}_j$ LEAD TO STIFF PROBLEMS

- STEADY-STATE APPROXIMATION (SS) - CONSIDER THE SYSTEM $R \xrightarrow{P} X$, $X \xrightarrow{d} B$, THEN

($R \xrightarrow{P} X$: PRODUCTION OF X; $X \xrightarrow{d} B$: DEPLETION OF X)

$$\frac{\partial Y_R}{\partial t} + \underline{v} \cdot \nabla Y_R = -\frac{1}{\rho} \nabla \cdot (\rho Y_R \underline{V_R}) + W_R k_p \frac{Y_R}{W_R}$$

$$\frac{\partial Y_B}{\partial t} + \underline{v} \cdot \nabla Y_B = -\frac{1}{\rho} \nabla \cdot (\rho Y_B \underline{V_B}) + W_B k_d \frac{Y_X}{W_X}$$

$$\frac{\partial Y_X}{\partial t} + \underline{v} \cdot \nabla Y_X = -\frac{1}{\rho} \nabla \cdot (\rho Y_X \underline{V_X}) + W_X k_p \frac{Y_R}{W_R} - W_X k_d \frac{Y_X}{W_X}$$

IF $\Gamma_j = \frac{Y_j}{W_j} = \frac{[j]}{\rho}$ IS DEFINED, THEN, THESE CONSERVATION EQUATIONS REDUCE TO:

$$\mathcal{L}(\Gamma_R) = -k_p \Gamma_R$$
$$\mathcal{L}(\Gamma_B) = k_d \Gamma_X$$
$$\mathcal{L}(\Gamma_X) = k_p \Gamma_R - k_d \Gamma_X$$
$$O(1/t_m) \quad O(1/t_p) \quad O(1/t_d)$$

WITH $\mathcal{L} = \frac{\partial}{\partial t} + \underline{v} \cdot \nabla + \frac{1}{\rho} \nabla \cdot (\rho \underline{V})$

$t_m$ = FLUID-MECHANICAL TIME (DIFFUSION, CONVECTION, ACCUMULATION)

WITH $t_p$ = PRODUCTION TIME, $t_d$ = DEPLETION TIME

IF $t_p \sim t_d \ll t_m$ OR $t_d \ll t_p \sim t_m \rightarrow$ X IS IN STEADY STATE, IN THAT THE TRANSPORT TERMS IN THE TRANSPORT EQUATION OF $Y_X$ CAN BE NEGLECTED, WHICH GIVES

$$\Gamma_R k_p = k_d \Gamma_X \rightarrow \boxed{Y_X = W_X \left(\frac{k_p}{k_d}\right) \frac{Y_R}{W_R}} \rightarrow \boxed{\frac{D[X]}{Dt} = \sum_{j=1}^{M} (\nu_{xj}'' - \nu_{xj}') \dot{\omega}_j = 0} \quad \text{FOR X IN SS}$$

THE ORIGINAL SET OF TWO REACTIONS CAN THEN BE REDUCED TO $R \rightarrow B$, WITH A RATE OF REACTION $\dot{\omega}_d = \dot{\omega}_p = k_p [R] = k_d [X]$. WHEN $t_p \gg t_d$, WITH $t_d \sim t_m$, THEN $\frac{t_d}{t_p} \sim \frac{k_p}{k_d} \ll 1$, AND $\Gamma_X \ll 1 \Rightarrow$ THE SPECIES WITH SMALL CONCENTRATIONS TEND TO BE IN STEADY STATE.

- PARTIAL-EQUILIBRIUM APPROXIMATION (PEA)

THE PEA IS APPLIED TO REACTIONS INSTEAD OF SPECIES (LIKE THE SS). CONSIDER THE SYSTEM

$F + O \xrightarrow{1} X$
$X + O \underset{2}{\rightleftharpoons} P$

$$\rho \mathcal{L}(\Gamma_F) = -\dot{\omega}_1 = -k_1 [F][O]$$
$$\rho \mathcal{L}(\Gamma_O) = -\dot{\omega}_1 - \dot{\omega}_2 = -k_1 [F][O] - k_{2f} [X][O] + k_{2b} [P]$$
$$\rho \mathcal{L}(\Gamma_X) = \dot{\omega}_1 - \dot{\omega}_2 = k_1 [F][O] - k_{2f} [X][O] + k_{2b} [P]$$
$$\rho \mathcal{L}(\Gamma_P) = \dot{\omega}_2 = +k_{2f} [X][O] - k_{2b} [P]$$

CHARACTERISTIC TIME SCALES: $t_1 \sim \left(k_1 [O]_0\right)^{-1}$, $t_{2f} \sim \left(k_{2f} [O]_0\right)^{-1}$, $t_{2b} \sim k_{2b}^{-1}$, $t_M$

IF $t_{2f} \sim t_{2b} \ll t_M$ AND $t_{2f} \sim t_{2b} \ll t_1 \Rightarrow$ THE FORWARD AND BACKWARD RATES OF 2 ARE ALMOST

EQUAL AND MUCH LARGER THAN THE TRANSPORT OF THE INVOLVED REACTANTS, SO THAT

$$\boxed{k_{2f} C_x C_o \approx k_{2b} C_p}$$ , HOWEVER, THIS DOES NOT MEAN THAT $\dot{\omega}(\Gamma_p) = 0$.

IN FACT, $\omega_{2f} - \omega_{2b}$ COULD BE OF THE SAME ORDER AS $\rho \dot{\omega}[\Gamma_p]$. TO AVOID THE RESULTING STIFFNESS, THE DIFFERENCE $\omega_{2f} - \omega_{2b}$ SHOULD BE ELIMINATED FROM THE CONSERVATION EQUATIONS, USING, FOR INSTANCE

$$\left.\begin{aligned} \rho \dot{\omega}(\Gamma_F) &= -k_1 [F][O] \\ \rho[\dot{\omega}(\Gamma_O) + \dot{\omega}(\Gamma_P)] &= -k_1 [F][O] \\ \rho[\dot{\omega}(\Gamma_b) - \dot{\omega}[\Gamma_x]) &= -2k_1 [F][O] \\ k_{2f}[O][X] &= k_{2b}[P] \end{aligned}\right\}$$

## $H_2$-$O_2$ CHEMISTRY

- CHARATERISTICS OF $H_2$ : LIGHT WEIGHT ($W_{H_2} = 2\,g/mol$) AND THERGFORE LARGE DIFFUSION COEFFICIENT ($D_{H_2} = 7.8 \cdot 10^{-5}\,m^2/s$ IN AIR, COMPARE TO $D_{O_2} = 1.9 \cdot 10^{-5}\,m^2/s$ IN AIR) ASSOCIATED WITH THIS LIGHT WEIGHT IS A SMALL LEWIS NUMBER $Le_{H_2} \sim 0.3$ FOR COMBUSTION OF $H_2$ IN $O_2$. → SEE EXPLOSION LIMITS IN FIG 4 AND FIG 5
- AT THE 3RD EXPLOSION LIMIT AND ABOVE, FORMATION OF $H_2O_2$ THROUGH STEP 17 $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$, FOLLOWED BY GENERATION OF ACTIVE RADICALS BY 16b $H_2O_2 + M \rightarrow OH + OH + M$, IS AN IMPORTANT ACCELERATOR OF COMBUSTION. THE HYDROPEROXY RADICAL IS MAINLY FORMED BY $H + O_2 + M \rightarrow HO_2 + M$.
- AT THE CROSSOVER TEMPERATURES $T_c$, THE RATES OF 1 $H + O_2 \rightarrow OH + O$ AND 10 $H + O_2 + M \rightarrow HO_2 + M$ ARE EQUAL. IN PARTICULAR, $T_c \sim 1000K$ AT 1 ATM AND $T_c \sim 1500K$ AT 50 ATM. THIS CROSSOVER TEMPERATURE IS LOW IN COMPARISON WITH HYDROCARBON COMBUSTION → SAFETY PROBLEMS.
- THE FIRST EXPLOSION LIMIT IS DOMINATED BY HETEROGENEOUS REACTIONS AT THE WALLS. THESE RATES ARE VERY UNCERTAIN AND SURFACE-SPECIFIC.
- THE $H_2/O_2$ MECHANISM IS A SUBMECHANISM FOR THE COMBUSTION OF HYDROCARBONS. ⇒ NUMBERS ARE HEREAFTER REFERRED TO TABLE 1.
- ABOVE THE SECOND EXPLOSION LIMIT, THE COMBUSTION OF $H_2/O_2$ MIXTURES IS DESCRIBED BY THE COMPETITION BETWEEN 1 $H + O_2 \rightarrow OH + O$ BRANCHING (RADICAL BUILD UP) AND 10 $H + O_2 + M \rightarrow HO_2 + M$ TERMINATION (HEAT RELEASE)

THE TEMPERATURE AT WHICH BOTH RATES ARE EQUAL IS THE CROSSOVER TEMPERATURE $T_c$. FOR $T > T_c$, 1 WINS OVER 10 AND THE CHAIN CARRIERS MULTIPLY. FOR $T < T_c$, 10 WINS OVER 1, AND CHEMICAL REACTION IS TOO SLOW. → SEE CROSSOVER LINE IN FIG 4 AND FIG 5

- FALL-OFF EFFECT : THIS EFFECT IS RELATED TO THE PRESSURE DEPENDENCE OF THE REACTION RATE OF THE RECOMBINATION REACTIONS. TO MODEL THIS EFFECT, USE IS TYPICALLY MADE OF THE LINDEMANN MECHANISM :

$$\left.\begin{aligned} H + O_2 + M &\underset{2}{\overset{1}{\rightleftharpoons}} HO_2^* + M \\ HO_2^* &\xrightarrow{2} HO_2 \end{aligned}\right\}$$ WITH $HO_2^*$ AN INTERMEDIATE EXCITED SPECIES.

$[M] = \frac{P}{R^0 T}$ COLLIDER'S CONCENTRATION

THEN $\frac{d[HO_2^*]}{dt} = \omega_{1f} - \omega_{1b} - \omega_2 = k_{1f}[H][O_2][M] - k_{1b}[HO_2^*][M] - k_2[HO_2^*]$

IF $[HO_2^*]$ IS ASSUMED TO BE IN STEADY STATE ($t_2 \ll t_1$), THEN $\frac{d[HO_2^*]}{dt} = 0$ AND $[HO_2^*] = \frac{k_{1f}[H][O_2][M]}{k_{1b}[M] + k_2}$

THE MASS PRODUCTION OF $HO_2$ IS THEN GIVEN BY $\dot{w}_{HO_2} = W_{HO_2}\omega_2 = W_{HO_2} k_2 [HO_2^*] = W_{HO_2} \tilde{k} [H][O_2][M]$

WITH $$\boxed{\tilde{k} = \frac{k_{1f}}{\frac{k_{1b}[M]}{k_2} + 1} = \frac{k_{1f}}{\frac{k_{1f}[M]}{k_c k_2} + 1}}$$ THE TRUE RATE CONSTANT OF $HO_2$ PRODUCTION, WHERE $k_{c_1} = \frac{k_{1f}}{k_{2b}}$ IS THE EQUILIBRIUM CONSTANT.

- FOR LOW PRESSURES, $\frac{k_{1f}[M]}{k_{c_1}k_2} \ll 1 \rightarrow \dot{w}_{HO_2} = w_{HO_2}\left(k_{1f}^{k_0}\right)[H][O_2][M]$ → THE CHEMICAL REACTION ↑ IS TRIMOLECULAR.
- FOR HIGH PRESSURES, $\frac{k_{1f}[M]}{k_{c_1}k_2} \gg 1 \rightarrow \dot{w}_{HO_2} = w_{HO_2}\left(k_{c_1}^{k_\infty}\, k_2\right)[O_2][H]$ → THE CHEMICAL REACTION ↑ IS BIMOLECULAR.

PRESSURE CUT-OFF ≈ 50 bar

SINCE THE TRUE RATE $\tilde{k} = \frac{k_0'}{1+\frac{[M]k_0}{k_\infty}}$ IS ALWAYS LOWER THAN THAT PREDICTED SOLELY BY $k_0$ OR $k_\infty$,

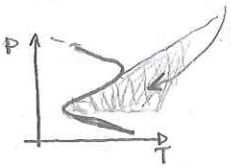
IT IS SAID TO "FALL-OFF". HOWEVER, THE LINDEMANN TRANSITION TENDS TO BE TOO ABRUPT, SO THAT IT IS CUSTOMARY TO USE A TRANSITION MODEL LIKE THE ONE PROPOSED BY TROE:

$$\tilde{k} = \frac{k_0}{1+\frac{[M]k_0}{k_\infty}} F_c \left\{1+\left[(0.75-1.27\log F_c)^{-1}\ln\left(\frac{k_0[M]}{k_\infty}\right)\right]^2\right\}^{-1} \quad (11\text{-PARAMETER})$$

WITH $F_c = a e^{-T/T_1} + (1-a)e^{-T/T_2} + b e^{-T_3/T}$

## HYDROGEN-OXYGEN AUTOIGNITION:

1. OVERALL DESCRIPTION AT THE SECOND LIMIT AND ABOVE CROSSOVER:




3 STAGES:

i) INITIATION: AT VERY HIGH TEMPERATURES, THE REVERSE OF THE RECOMBINATION STEPS 5, 6 AND 7 PRODUCE RADICALS:

5b $H_2 + M \rightarrow H + H + M$

6b $H_2O + M \rightarrow H + OH + M$ $\quad T \gtrsim 2500\,K$

7b $O_2 + M \rightarrow O + O + M$

HOWEVER, IN COMBUSTION INITIAL TEMPERATURES ARE NOT HIGH ENOUGH FOR DISSOCIATION TO OCCUR. INSTEAD, THE MAIN INITIATION STEP IS

12b $H_2 + O_2 \rightarrow HO_2 + H$

WITH AN ACTIVATION ENERGY $E = 200\ kJ/mol$, CAUSING THE STEP TO BE SLOW BUT FASTER THAN ANY OTHER INITIATION PATH.

SEE FIG 6

ii) CHAIN BRANCHING AND PROPAGATION: AFTER INITIATION, THE HYDROGEN OXIDATION CHAIN IS FOLLOWED BY A CHAIN BRANCHING PROCESS IN WHICH 2 H RADICALS ARE GENERATED PER H ATOM CONSUMED:

CHAIN PROPAGATION →

1f: $H + O_2 \xrightarrow{1} OH + O$

2f: $H_2 + O \xrightarrow{2} OH + H$

3f: $H_2 + OH \xrightarrow{3} H_2O + H$

CONSIDERING OH AND O IN STEADY STATE, THE BRANCHING IS CONTROLLED BY 1 WITH A RATE $2\dot{w}_1$

$[OH] = w_1 + w_2 - w_3 = 0$
$[O] = w_1 - w_2 = 0$
$[H] = -w_1 + w_2 + w_3 = 2w_1$

$w_1 = w_2$
$w_3 = 2w_1$

iii) CHAIN TERMINATION: THE H-RADICALS AND THE REMAINING O AND OH RADICALS ARE CONSUMED IN THE RECOMBINATION REACTIONS, DURING WHICH HEAT IS RELEASED:

5f: $H + H + M \rightarrow H_2 + M$
6f: $H + OH + M \rightarrow H_2O + M$
7f: $O + O + M \rightarrow O_2 + M$
8f: $H + O + M \rightarrow OH + M$
9f: $O + OH + M \rightarrow HO_2 + M$

BUT ALL THESE TEND TO BE SLOWER THAN THE TERMINATION STEP 10

10f: $H + O_2 + M \rightarrow HO_2 + M$

AUTOIGNITION CAN THEN BE DESCRIBED BY A QUALITATIVE MODEL

$$\Rightarrow \frac{d[H]}{dt} = k_1[H_2][O_2] + 2k_1[H][O_2] - k_{10}[H][O_2][M]$$

$[H] = [H]_0$ AT $t = 0$

WHICH GIVES THAT $t_I \sim t_B \ln\left[\frac{t_B}{t_I} + \frac{[H]_0}{[H_2]_0}\right]$

SEE FIG 7

INITIATION TIME

$$\begin{cases} t_I = \left(k_{12}[O_2]_0\right)^{-1} \\ t_B = \left(2k_{1f}[O_2]_0\right)^{-1} \end{cases}$$

→ BRANCHING TIME

- REDUCED CHEMISTRY FOR HYDROGEN AUTOIGNITION (DEL ÁLAMO, SÁNCHEZ & WILLIAMS, 2006)

| | | |
|---|---|---|
| 1 | $H_2+O_2 \rightarrow HO_2+H$ | INITIATION |
| 2 | $H+O_2 \rightarrow OH+O$ | BRANCHING |
| 3 | $O+H_2 \rightarrow OH+H$ | BRANCHING |
| 4 | $OH+H_2 \rightarrow H_2O+H$ | PROPAGATION |
| 5 | $H+O_2+M \rightarrow HO_2+M$ | TERMINATION |

IN THIS DESCRIPTION, $HO_2$ IS NOT CONSUMED AND $H_2O_2$ DOES NOT PARTICIPATE. THESE RESTRICTIONS WILL LEAD TO A LOW TEMPERATURE LIMIT BELOW WHICH THE MECHANISM IS INAPPLICABLE. IN PARTICULAR, THE MECHANISM FAILS AT AND BELOW THE TEMPERATURE OF CROSSOVER. IT DOES NOT ACCOUNT EITHER FOR INITIATION BY DISSOCIATION. FOR $\phi \ll 1$ IT BECOMES ENDOTHERMIC BECAUSE OF STEP 1.

BY IMPOSING O AND OH STEADY STATE (VALID FOR FUEL-RICH AND NEAR STOICHIOMETRIC MIXTURES), STEPS 2, 3 AND 4 REDUCE TO $3H_2+O_2 \rightarrow 2H_2O+2H$ $\left((3)+2\times(4)+(2)\right)$ WITH A RATE $2\omega_2$. IN THIS WAY, IMPOSING O AND OH STEADY STATES REDUCES THE 5-STEP MECHANISM TO A 3-STEP MECHANISM COMPOSED OF 1, 5 AND $3H_2+O_2 \rightarrow 2H_2O+2H$. IN MATHEMATICAL TERMS:

$$\left.\begin{aligned}[OH] &= \omega_2+\omega_3-\omega_4=0\\ [O] &= \omega_2-\omega_3=0\end{aligned}\right\} \quad \boxed{\omega_2=\omega_3 \;\; \omega_4=2\omega_2} \rightarrow \text{THEN } k_3[O][H_2]=[H][O_2]k_2 \rightarrow [O]=2\frac{[H][O_2]}{[H_2]}\frac{k_2}{k_3}$$

$$\text{AND } 2k_2[H][O_2]=[OH][H_2]k_4 \rightarrow [OH]=\frac{2k_2}{k_4}\frac{[H][O_2]}{[H_2]}$$

WITH $[O]$ AND $[OH]$ SMALL SINCE $k_3 \gg k_2$ AND $k_4 \gg k_2$

THEN THE SPECIES CONSERVATION EQUATION FOR $[H]$ READS

$$\frac{d[H]}{dt}=\omega_1+2\omega_2-\omega_5=k_1[H_2][O_2]+2k_2[H][O_2]-k_3[H][O_2][M] \quad (*)$$

SUBJECT TO $[H]=0$ AT $t=0$

ISOCHORIC SYSTEMS ($\rho$=CONST)

IF CHANGES IN TEMPERATURE ARE SMALL, AS OFTEN IS TRUE DURING INDUCTION, AND IF THE REACTANT DEPLETION PRIOR TO IGNITION IS NEGLECTED, THEN (*) BECOMES LINEAR AND INTEGRABLE ANALYTICALLY. THE RESULTING EVOLUTION OF $[H]$ IN TIME IS CONTINUOUS AND A CRITERION MUST BE INTRODUCED TO SPECIFY AN AUTOIGNITION TIME. ONCE THE CHEMISTRY BEGINS TO ACCELERATE, RECOMBINATION REACTIONS BECOME IMPORTANT, CAUSING RADICAL CONCENTRATIONS TO REACH A MAXIMUM VALUE. A THRESHOLD VALUE FOR RADICAL CONCENTRATIONS AT IGNITION CAN BE BASED ON THE REVERSE OF 2 OR 3 BECOMING IMPORTANT. A PLAUSIBLE DEFINITION OF AUTOIGNITION TIME IS THE ACHIEVEMENT OF PARTIAL EQUILIBRIUM OF REACTION 2:

$$\omega_{2f}=\omega_{2b} \rightarrow [OH][O]k_{2b}=[H][O_2]k_{2f} \rightarrow \frac{[OH][O]}{[H][O_2]}=k_{2c}$$

, WITH $k_{2c}$ THE EQ CONSTANT OF 2.

SUBSTITUTING THE $[O]$ AND $[OH]$ FROM STEADY-STATE CONSIDERATIONS IN THE ABOVE EXPRESION, AND USING IT IN (*) THEN EXPRESSIONS FOR THE AUTOIGNITION TIME

$$t_R=\frac{1}{(2k_2-k_5[M])[O_2]}\ln\left[\frac{k_{2c}k_3k_4(2k_2-k_5[M])[H_2]}{2k_1k_2^2[O_2]}\right]$$

IS OBTAINED FOR RICH MIXTURES

SEE FIG 9a AND a3

AN ANALYSIS OF THE SAME TYPE FOR FUEL-LEAN CONDITIONS, IN WHICH ONLY THE H ATOM IS IN STEADY STATE, LEADS TO:

USE $t_i=t_R+t_L$

$$t_L=\frac{2(k_2+k_5[M])\cdot\ln\left\{\left[4k_{2c}k_3k_4\left(\sqrt{2k_4}+\sqrt{k_3}\right)[H_2]\right]/\left[k_1k_2\left(\sqrt{2k_4}+2\sqrt{k_3}\right)[O_2]\right]\right\}}{[H_2]\left\{\left[4k_3k_4\left(2k_2^2+k_2k_5[M]-k_5^2[M]^2\right)+\left(k_3+k_4\right)^2k_5^2[M]^2\right]^{1/2}-(k_3+k_4)k_5[M]\right\}}$$

- CHEMISTRY REDUCTION FOR GENERAL $H_2$ - COMBUSTION PROBLEMS (BOIVIN, PCI 2010).

THE REDUCTION BEGINS BY NOTING THAT THE FLAME STRUCTURE AND AUTOIGNITION CALCULATIONS REVEAL THAT MANY ELEMENTARY REACTIONS HAVE A NEGLIGIBLE CONTRIBUTION TO THE REACTION PROCESS. TWELVE ELEMENTARY REACTIONS SUFFICE TO DESCRIBE PREMIXED AND NONPREMIXED FLAMES, AUTOIGNITION AND DETONATIONS UNDER CONDITIONS OF PRACTICAL INTEREST:

1. $H+O_2 \rightleftharpoons OH+O$
2. $H_2+O \rightleftharpoons OH+H$
3. $H_2+OH \rightleftharpoons H_2O+H$
4. $H+O_2+M \rightarrow HO_2+M$
5. $HO_2+H \rightarrow 2OH$
6. $HO_2+H \rightleftharpoons H_2+O_2$
7. $HO_2+OH \rightarrow H_2O+O_2$
8. $H+OH+M \rightleftharpoons H_2O+M$
9. $2H+M \rightleftharpoons H_2+M$
10. $2HO_2 \rightarrow H_2O_2+H$
11. $HO_2+H_2 \rightarrow H_2O_2+H$
12. $H_2O_2+M \rightarrow 2OH+M$

SUBSET — SUFFICIENT FOR

$\{1, 2, 3, 4f, 5f, 6f, 7f\} \Rightarrow$ LEAN DEFLAGRATIONS

$\{1, 2, 3, 4f, 5f, 6f, 7f, 8f, 9f\} \Rightarrow$ STOICHIOMETRIC TO RICH DEFLAGRATIONS AND NONPREMIXED FLAMES

$\{1, 2, 3, 4, 6b, 8, 9\} \Rightarrow$ AUTOIGNITION AND DETONATIONS.

EVERYTHING THAT INVOLVES LOW TEMPERATURES (NEAR CROSSOVER) OR HIGH PRESSURES, NEEDS TO INCLUDE THE ALTERNATE CHAIN PATH GIVEN BY 12f.

STEADY STATES — SUFFICIENT FOR

$\{OH, O \text{ AND } HO_2\}$ — DEFLAGRATIONS

$\{OH, O, H \text{ AND } HO_2\}$ — VERY LEAN DEFLAGRATIONS

$\{HO_2\}$ BETTER THAN $\{HO_2, OH\}$ AND BETTER THAN $\{HO_2, OH, O\}$ — NON-PREMIXED FLAMES, 20% ERROR IN $\varphi_{EXT}$

$\{OH, O\}$ — STOICHIOMETRIC TO FUEL RICH AUTOIGNITION

$\{H\}$ — VERY LEAN AUTOIGNITION

$\{HO_2\}$ — AUTOIGNITION BELOW CROSSOVER

$\{H_2O_2\}$ — ALMOST ALWAYS EXCEPT FOR AUTOIGNITION BELOW CROSSOVER.

WHEN O, OH AND $H_2O_2$ ARE TAKEN IN STEADY STATE, THE 3-STEP MECHANISM

BRANCHING
RECOMBINATION
INITIATION

$$3H_2 + O_2 \overset{I}{\rightleftharpoons} 2H_2O + 2H$$
$$H + H + M \overset{II}{\rightleftharpoons} H_2 + M$$
$$H_2 + O_2 \overset{III}{\rightleftharpoons} HO_2 + H$$

$$\omega_I = \omega_{1f} - \omega_{1b} + \omega_{5f} + \omega_{10f} + \omega_{11f}$$
$$\omega_{II} = \omega_{4f} + 2\omega_{8f} - \omega_{8b} + \omega_{4f} - \omega_{9b} - \omega_{10f} - \omega_{11f}$$
$$\omega_{III} = \omega_{4f} - \omega_{5f} - \omega_{6f} + \omega_{6b} - \omega_{7f} - 2\omega_{10f} - \omega_{11f}$$

IS OBTAINED $\Rightarrow$ GIVES 12% ERROR IN PROPAGATION VELOCITIES (ERROR DECREASES FOR INCREASING PRESSURE), 50K ERROR IN FLAME TEMPERATURE, AND TOO SHORT AUTOIGNITION TIMES FOR LEAN MIXTURES. (ERROR ASSOCIATED WITH O AND OH STEADY STATES, SINCE O AND OH ALSO CONTROL AUTOIGNITION IN LEAN MIXTURES).

$\Rightarrow$ THIS CAN BE SOLVED BY MODIFYING $\omega_I$, $\omega_{II}$ AND $\omega_{III}$.

SEE FIG 12

## $CH_4$-$O_2$ CHEMISTRY:

- A 4-STEP REDUCED MECHANISM CAN BE OBTAINED BY USING STEADY STATE FOR O, OH, $HO_2$, $CH_3$, $CH_2O$ AND CHO, AND PARTIAL EQUILIBRUM FOR STEPS 2 AND 3 (PETERS + WILLIAMS, CSF 1987):

SUMMING UP THE FASTEST REACTIONS IN THE $C_1$ CHAIN:

| | | |
|---|---|---|
| 11 | $CH_4 + H \longrightarrow CH_3 + H_2$ | AND TAKING PARTIAL EQUILIBRIUM IN |
| 13 | $CH_3 + O \longrightarrow CH_2O + H$ | $H + OH \rightleftharpoons O + H_2$ |
| 17 | $CH_2O + H \longrightarrow CHO + H_2$ | $H + H_2O \rightleftharpoons OH + H_2$ |
| 22 | $CHO + M \longrightarrow CO + H + M$ | |
| | $CH_4 + O \xrightarrow{w_{11}} CO + 2H_2$ | THEN I: $CH_4 + 2H + H_2O \longrightarrow CO + 4H_2$ IS OBTAINED. |

SIMILARLY, THE COMBINATION 10 $CO + OH \rightleftharpoons CO_2 + H$; 3 $H + H_2O \rightleftharpoons OH + H_2$ } YIELDS II: $CO + H_2O \rightleftharpoons CO_2 + H_2$ WATER-GAS SHIFT REACTION

AND ALSO: 5 $O_2 + H + M \longrightarrow HO_2 + M$; 9 $OH + HO_2 \longrightarrow H_2O + O_2$; 3b $H + H_2O \longrightarrow OH + H_2$ } YIELDS III: $2H + M \longrightarrow H_2 + M$

FINALLY 1 $O_2 + H \rightleftharpoons OH + O$; 2 $O + H_2 \rightleftharpoons OH + H$; 3 $OH + H_2 \rightleftharpoons H_2O + H$ } GIVES IV: $O_2 + 3H_2 \rightleftharpoons 2H_2O + 2H$

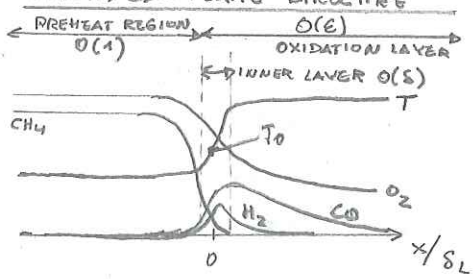
⇒ 4-STEP MECHANISM

| | | |
|---|---|---|
| I: | $CH_4 + 2H + H_2O \longrightarrow CO + 4H_2$ | BREAKING |
| II: | $CO + H_2O \rightleftharpoons CO_2 + H_2$ | WATER-GAS SHIFT |
| III: | $H + H + M \longrightarrow H_2 + M$ | BREAKING |
| IV: | $O_2 + 3H_2 \longrightarrow 2H_2O + 2H$ | BRANCHING |

IN THIS MECHANISM, ONLY THE KINETIC DATA OF FOUR ELEMENTARY REACTIONS APPEARS (SEE REF. PAPER):

| | | |
|---|---|---|
| FOR I: | 11: | $CH_4 + H \longrightarrow CH_3 + H_2$ |
| FOR II: | 10: | $CO + OH \rightleftharpoons CO_2 + H$ |
| | 3: | $H + H_2O \rightleftharpoons OH + H_2$ |
| FOR III: | 5: | $H + O_2 + M \longrightarrow HO_2 + M$ |
| FOR IV: | 1: | $H + O_2 \longrightarrow OH + O$ |

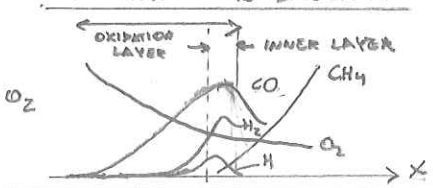
- PREMIXED-FLAME STRUCTURE




• IN THE FUEL-CONSUMPTION (INNER) LAYER THE FUEL IS ATTACKED BY H RADICALS IN THE CHAIN-BREAKING REACTION I, WHICH ARE FORMED THROUGH THE BRANCHING STEP IV. IN THIS LAYER THERE IS A CHARACTERISTIC CROSSOVER TEMPERATURE THAT IS REPRESENTATIVE OF THE CROSSING EFFECTS OF BRANCHING (1) AND CHAIN BREAKING (5, 11). THIS TEMPERATURE IS TYPICALLY 500-700 K LARGER THAN IN $H_2$-$O_2$ FLAMES. THIS LAYER HAS A THICKNESS $\ell_\delta \sim \delta \cdot \delta_L \sim 0.1 \cdot 175 \mu m \sim 18 \mu m$ WHICH DECREASES WITH INCREASING PRESSURE ($\delta \sim 0.03$ AT 30 ATM).

• IN THE OXIDATION LAYER, REACTIONS II, III AND IV ARE IMPORTANT, HERE THE $H_2$ AND CO ARE OXIDIZED TO $H_2O$ AND $CO_2$. THIS LAYER HAS A THICKNESS $\ell_\varepsilon \sim \varepsilon \delta_L \sim 3\ell_\delta \sim 60 \mu m$.

- DIFFUSION FLAME STRUCTURE




⇒ THE OXIDATION LAYER IS LOCATED ON THE OXIDIZER SIDE. OUTSIDE THE OXIDATION AND INNER LAYERS, THE CONCENTRATIONS OF ALL SPECIES EXCEPT $CH_4$, $CO_2$, $N_2$, $O_2$ AND $H_2O$ ARE ZERO ⇒ CHEMICALLY INERT ZONES.

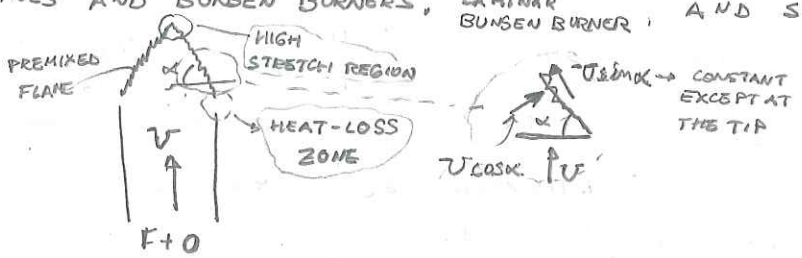
# ASYMPTOTIC STRUCTURES IN COMBUSTION

- COMBUSTION IS CHARACTERIZED BY CHEMICAL REACTIONS WITH LARGE ACTIVATION-ENERGY BARRIERS. IN PARTICULAR, THE OVERALL ACTIVATION ENERGY IN COMBUSTION SYSTEMS IS TYPICALLY MUCH LARGER THAN THE CHEMICAL HEAT RELEASED BY REACTIONS. THIS CAN BE EXPRESSED BY NOTICING THAT THE RATIO $\frac{E_a}{R^0 T_f} \gg 1$ IS TYPICALLY LARGE, WITH $E_a$ THE OVERALL ACTIVATION ENERGY AND $T_f$ THE CHARACTERISTIC FLAME TEMPERATURE. THAT $\frac{E_a}{R^0 T_f}$ IS A LARGE PARAMETER MEANS THAT THE OVERALL CHEMICAL RATE $\dot{w}$ TENDS TO BE HIGHLY SENSITIVE TO TEMPERATURE. IN PARTICULAR, IF $\dot{w} \sim \text{const.} \, e^{-\frac{T_a}{T}}$ FOR A VIGOROUSLY-BURNING FLAME, WITH $T_a = \frac{E_a}{R^0}$ THE ACTIVATION TEMPERATURE, THEN $\dot{w} \sim \text{const.} \cdot e^{-\frac{T_a}{T_f}\left(\frac{T_f}{T} - 1 + 1\right)} \sim \text{const.} \cdot e^{-\frac{T_a}{T_f}} e^{\frac{T - T_a}{T_f}\left(\frac{T_f - T}{T}\right)}$. THEREFORE, TEMPERATURE VARIATIONS $\frac{T_f - T}{T_f} \sim O\left(\frac{T_f}{T_a}\right) \ll 1$ GENERATE ORDER-UNITY VARIATIONS IN THE CHEMICAL-REACTION TERM.

- AS A RESULT OF THE HIGH SENSITIVITY OF CHEMICAL RATES TO TEMPERATURE, FLAMES ARE CONFINED TO VERY THIN REGIONS (OF ORDER $\lesssim 100\,\mu m$) IN WHICH (THE TEMPERATURE ATTAINS HIGH VALUES AND THE RESIDENCE TIME IS LARGE ENOUGH) THAT THERE IS SUFFICIENT TIME FOR THE REACTANTS TO BE DEPLETED BY CHEMICAL REACTIONS. THIS THIN REGIONS REPRESENT CHEMICAL BOUNDARY LAYERS.
- HISTORICALLY, THERE HAVE BEEN NUMEROUS DEVELOPMENTS ON THE TREATMENT OF FLAMES USING ASYMPTOTIC ANALYSES TO PALLIATE THE SINGULAR CHARACTER OF THE PROBLEM IN HYDRODYNAMIC SCALES. THESE DEVELOPMENTS INCLUDED DAMKÖHLER-NUMBER ASYMPTOTICS (DNA, SEE WORKS BY FENDELL, WILLIAMS AND OTHERS), LARGE ACTIVATION-ENERGY ASYMPTOTICS (AEA, SEE WORKS BY ZEL'DOVICH, LIÑÁN, BUCKMASTER, WILLIAMS AND OTHERS) AND RATE-RATIO ASYMPTOTICS (RRA, SEE WORKS BY PETERS, SESHADRI, WILLIAMS AND OTHERS). THE ABSTRACTIONS OBTAINED FROM AEA RESULTS (LIÑÁN, 1974) WERE LATER USED TO, FOR INSTANCE, CONCEPTUALIZE FLAMELET MODELS IN TURBULENT COMBUSTION (PETERS, 1983). AEA ANALYSES HAVE MADE TRADITIONAL USE OF SINGLE-STEP CHEMISTRY, WHILE RRA TECHNIQUES INTRODUCED A MORE POWERFUL APPARATUS TO OBTAIN ASYMPTOTIC STRUCTURES WITH MULTI-STEP CHEMISTRY.

## 1. ACTIVATION-ENERGY ASYMPTOTIC ANALYSES OF PREMIXED FLAMES

- IN PREMIXED COMBUSTION, THE FUEL AND OXIDIZER ENTER IN THE COMBUSTION CHAMBER ALREADY MIXED, SUCH INERT PREMIXING CAN ONLY BE ATTAINED BELOW CERTAIN TEMPERATURE (i.e. THE CROSSOVER TEMPERATURE), BELOW WHICH CHAIN BRANCHING REACTIONS LEADING TO AUTOIGNITION ARE NEGLIGIBLE. EXAMPLES OF PREMIXED COMBUSTORS INCLUDE LEAN-PREMIXED-PREVAPORIZERS FOR GAS TURBINES, SPARK-IGNITION ENGINES AND BUNSEN BURNERS, → SHOW VIDEO OF LAMINAR BUNSEN BURNER, AND SPHERICAL COMBUSTION VESSELS.




$S_L^0 = U \cos\alpha$ LAMINAR PREMIXED-FLAME VELOCITY.

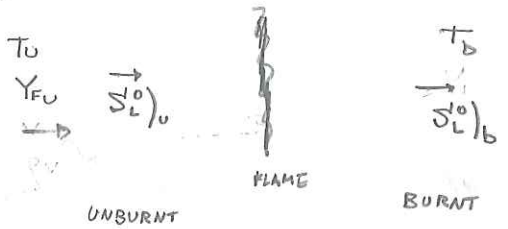
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PREMIXED FLAMES PROPAGATE WITH A SPEED THAT IS MAINLY A FUNCTION OF THE MIXTURE COMPOSITION AND THE THERMOCHEMISTRY. IF $\downarrow U$ THEN $\alpha$ NEEDS TO DECREASE UP TO THE FLASHBACK POINT $U < S_L^0$.

- PREMIXED FLAMES CAN BE STABILIZED IN FLAT POROUS BURNERS OR IN COUNTER FLOW BURNERS.

## FORMULATION FOR UNITY LEWIS NUMBERS AND SINGLE-STEP CHEMISTRY

(ZEL'DOVICH, FRANK-KAMENETSKII AND VON KÁRMÁN)




BECAUSE OF THERMAL EXPANSION $\rho_u > \rho_b$ AND $(S_L^0)_u < (S_L^0)_b$

CONSIDER A PLANAR PREMIXED FLAME PROPAGATING IN A MIXTURE IN WHICH THE FUEL IS THE DEFICIENT COMPONENT ($\phi < 1$). ASSUME A FIRST-ORDER IRREVERSIBLE CHEMICAL REACTION OF THE TYPE $F \longrightarrow P$, WITH A RATE $\dot{w}_F = \rho Y_F A e^{-\frac{E_a}{RT}}$. THE UNITY LEWIS NUMBER OF THE FUEL IS ASSUMED TO BE 1. IN THE LOW-MACH LIMIT, THE BACKGROUND PRESSURE REMAINS UNIFORM AND THE SPECIES AND ENTHALPY CONSERVATION EQUATIONS REDUCE TO:

$$\left.\begin{aligned} (1)\quad & \rho S_L^0 \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D_F \frac{dY_F}{dx}\right) + \rho Y_F A e^{-\frac{E_a}{RT}} \\ (2)\quad & \rho S_L^0 \frac{dT}{dx} = \frac{d}{dx}\left(\frac{\kappa}{c_p}\frac{dT}{dx}\right) + \frac{\rho q Y_F}{c_p} A e^{-\frac{E_a}{RT}} \end{aligned}\right\}$$

WHERE IT HAS BEEN ASSUMED THAT $c_p$ IS CONSTANT. IN THIS FORMULATION, $q$ IS THE CHEMICAL HEAT RELEASED PER UNIT MASS OF FUEL. NOTICE THAT CONTINUITY IMPOSES THAT $\rho S_L^0 =$ CONSTANT.

EQUATIONS (1) AND (2) SHOW THAT, FOR UNITY LEWIS NUMBERS, ($\frac{\kappa}{c_p} = \rho D_F$) THE EXCESS ENTHALPY $H = \frac{Y_F}{Y_{Fu}} + \frac{c_p(T-T_u)}{q Y_{Fu}}$ IS CONSERVED, SINCE

$$(3)\quad \rho S_L^0 \frac{dH}{dx} = \frac{d}{dx}\left(\rho D_F \frac{dH}{dx}\right),$$

WITH $H = 1$ AT $x \to -\infty$ ($Y_F = Y_{Fu}$, $T = T_u$), AND $H = 1$ AT $x \to +\infty$ ($Y_F = 0$, $T = T_u + \frac{q Y_{Fu}}{c_p} = T_b$ = ADIABATIC FLAME TEMPERATURE).

SO THAT $H = 1$ IS A SOLUTION OF (3).

THE EXCESS ENTHALPY IS THEN A CONSERVED SCALAR (AND A COUPLING FUNCTION), DEFINING THE DIMENSIONLESS VARIABLES

$$\Theta = \frac{c_p(T-T_u)}{q Y_{Fu}} = \frac{T-T_u}{T_b-T_u}, \qquad Y = \frac{Y_F}{Y_{Fu}}, \qquad \text{AND} \qquad \xi = \int_0^x \frac{\rho S_L c_p}{\kappa}\, dx,$$

EQUATIONS (1) AND (2) REDUCE TO

$$\left.\begin{aligned} (4)\quad & \frac{d\Theta}{d\xi} = \frac{d^2\Theta}{d\xi^2} + \Lambda Y e^{-\frac{\beta(1-\Theta)}{1-\alpha(1-\Theta)}} \\ (5)\quad & \text{AND} \quad \Theta + Y = 1 \end{aligned}\right\}$$

SUBJECT TO $\Theta \to 0$, $Y \to 1$ AS $\xi \to -\infty$

(6) $\Theta \to 1$, $Y \to 0$ AS $\xi \to +\infty$

WHERE USE HAS BEEN MADE OF $\frac{d}{dx} = \frac{d\xi}{dx}\frac{d}{d\xi} = \frac{\rho S_L c_p}{\kappa}\frac{d}{d\xi}$, $\frac{d}{dx}\left(\frac{\kappa}{c_p}\frac{d}{dx}\right) = \frac{(\rho S_L)^2 c_p}{\kappa}\frac{d^2}{d\xi^2}$

AND THE IDENTITY

$$e^{-\frac{E_a}{RT}} = e^{-\frac{T_a}{T}} = e^{-\frac{T_a}{T_b}\left(\frac{T_b}{T}-1+1\right)} = e^{-\frac{T_a}{T_b}\left(\frac{T_b-T_u-(T_b-T_u)\Theta+T_u-T_u}{\Theta(T_b-T_u)+T_u}\right)} e^{-\frac{T_a}{T_b}} =$$

$$= e^{-\frac{T_a}{T_b}} e^{-\frac{\beta(1-\Theta)}{1-\alpha(1-\Theta)}},$$

WITH $\beta = \frac{q Y_{Fu}}{c_p}\frac{E_a}{RT_b^2} \gg 1$ THE ZEL'DOVICH #

AND $\alpha = \frac{T_b-T_u}{T_b}$ A THERMAL-EXPANSION PARAMETER.

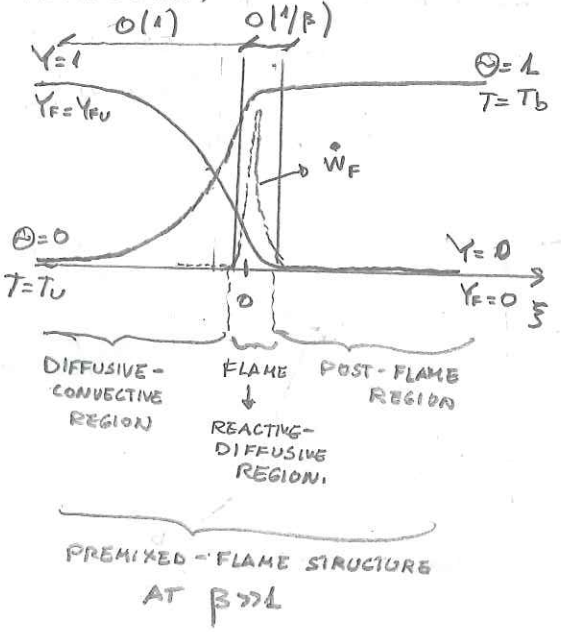
IN EQUATION (5), $\Lambda = \frac{\rho^2 D_F A}{(\rho S_L)^2} e^{-\frac{T_a}{T_b}}$ IS A DIMENSIONLESS PARAMETER (THE DAMKÖHLER NUMBER), WHICH FOR $\rho^2 D =$ CONSTANT REPRESENTS THE INVERSE OF A DIMENSIONLESS BURNING VELOCITY:

$$\frac{\beta}{\Lambda^{1/2}} = \frac{S_L^2}{\sqrt{D_F t_c}}, \qquad \text{WHERE} \quad t_c = \beta^{2-1} A^{-1} e^{\frac{T_a}{T_b}}$$

IS THE LOCAL CHEMICAL TIME OR FLAME-TRANSIT TIME

IN THIS PROBLEM, $\Lambda$ IS AN **EIGENVALUE**, IN THAT THERE IS ONLY 1 VALUE OF $\Lambda$ SUCH THAT (4) AND (5) SATISFY BOUNDARY CONDITIONS (6).

ADDITIONALLY, INSPECTION OF EQUATION (4) INDICATES THE FOLLOWING:




i) FOR $\xi$ LARGE AND NEGATIVE, $|\xi| \ll 1$ WITH $\xi < 0$, THERE EXISTS A REGION WHERE $1 - \Theta \gg \frac{1}{\beta}$, SO THAT THE TEMPERATURE IS LOW AND THE CHEMISTRY IS FROZEN

$\Rightarrow$ DIFFUSIVE-CONVECTIVE REGION $(Y \sim 1)$

ii) FOR $\xi$ LARGE AND POSITIVE, $\xi \gg 1$, THERE EXISTS A POST-FLAME REGION WHERE $\Theta \sim 1$ AND THE TEMPERATURE IS CLOSE TO THE ADIABATIC TEMPERATURE

$\Rightarrow$ POST-FLAME REGION $(Y \to 0)$

iii) FOR $\xi\beta = O(1)$, THERE EXISTS A REACTION ZONE IN WHICH THE AMOUNT OF FUEL DECAYS TO VALUES $Y \sim 1/\beta$ AND THE TEMPERATURE IS NEAR THE ADIABATIC TEMPERATURE $\Theta \sim 1 - 1/\beta$.

$\Rightarrow$ DIFFUSIVE-REACTIVE REGION $(Y \sim 1/\beta)$

- IN THE CONVECTIVE-DIFFUSIVE REGION, THE DOMINANT BALANCE IS

$$\frac{d\Theta}{d\xi} = \frac{d^2\Theta}{d\xi^2}$$ SUBJECT TO $\Theta \to 0$ AT $\xi \to -\infty$, WITH THE REACTION TERM EXPONENTIALLY SMALL

THEN $\Theta = e^{-\xi}$ AND $Y = 1 - e^{-\xi}$ IS THE SOLUTION IN THIS REGION.

THIS REGION IS TERMED THE PREHEAT REGION AND IT HAS A THICKNESS OF ORDER UNITY IN $\xi$ SCALES, OR EQUIVALENTLY, A THICKNESS OF ORDER $\delta_L^0 \sim D_f / S_L^0$ IN PHYSICAL UNITS.

- THE REACTIVE-DIFFUSIVE REGION HAS A THICKNESS OF ORDER $1/\beta$ IN $\xi$ SCALES, OR EQUIVALENTLY, A THICKNESS OF ORDER $\delta_f \sim \delta_L^0/\beta$ IN PHYSICAL UNITS. USING THE INNER VARIABLE $\eta = \beta\xi$, AND THE ASYMPTOTIC EXPANSIONS $\Theta = 1 - \tau/\beta$ AND $Y \sim \gamma/\beta$,

EQUATION (4) BECOMES $-\frac{1}{\beta}\frac{d\tau}{d\eta} = -\frac{d^2\tau}{d\eta^2} + \frac{\Lambda}{\beta^2}\tau e^{-\frac{\tau}{1-\alpha/\beta\tau}}$, WHICH BECOMES

$$\left.\begin{aligned} &\frac{d^2\tau}{d\eta^2} = \Lambda_0 \tau e^{-\tau} \\ &\tau \to 0 \text{ AT } \eta \to \infty \\ &\frac{d\tau}{d\eta} \to 1 \text{ AT } \eta \to -\infty \end{aligned}\right\}$$ WHEN $\Lambda = \beta^2\left(\Lambda_0 + \frac{\Lambda_1}{\beta} + \dots\right)$, WITH THE CONVECTION TERM BEING $1/\beta$ TIMES SMALLER IN THIS REGION.

THIS EQUATION CAN BE REWRITTEN AS $\frac{d^2\tau}{d\eta^2} = \frac{1}{2}\frac{d}{d\tau}\left(\frac{d\tau}{d\eta}\right)^2 = \Lambda_0 \tau e^{-\tau}$, WHICH CAN BE INTEGRATED ONCE TO GIVE

$$\frac{1}{2}\int_0^\tau \frac{d}{d\tau}\left(\frac{d\tau}{d\eta}\right)d\tau = \int_0^\tau \Lambda_0 \tau e^{-\tau} d\tau = \frac{1}{2}\left(\left.\frac{d\tau}{d\eta}\right|_\xi - \left.\frac{d\tau}{d\eta}\right|_{+\infty}\right)$$

THEN, AS $\xi \to -\infty$ $(\tau \to \infty)$, $\frac{d\tau}{d\eta} \to 1$ FROM THE MATCHING CONDITIONS AND THE BURNING EIGENVALUE BECOMES:

$$\Lambda_0 = \left[2\int_0^\infty \tau e^{-\tau} d\tau\right]^{-1} = \left[2\Gamma(2)\right]^{-1} = \frac{1}{2} \rightarrow \boxed{S_L^0 = \left\{\frac{2}{\beta^2} D_f A e^{-\frac{T_a}{T_b}}\right\}^{1/2} = \sqrt{\frac{D_f}{t_c}}} \qquad t_c = \frac{\delta_L^0}{S_L^0}$$

THE FLAME PROPAGATION VELOCITY IS A FUNCTION OF THE EQUIVALENCE RATIO $\phi$.

FOR A GLOBAL STEP OF THE TYPE $F + bO_2 \rightarrow P$, THE PARAMETERS

$b$ = STOICHIOMETRIC COEFFICIENT / MOLES OF $O_2$ REACTING PER MOL OF F

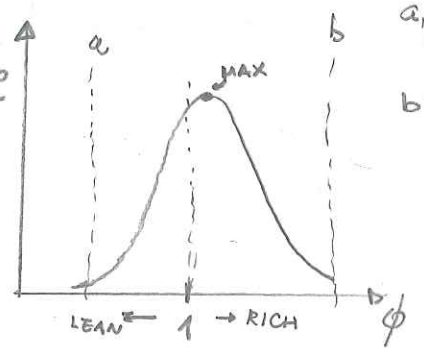
$s = \frac{b W_{O_2}}{W_F}$ MASS OF $O_2$ REACTING WITH THE UNIT MASS OF F. (EX: $b = \frac{1}{2}$, $s \sim 1.8$ FOR $H_2 - O_2$)

CAN BE DEFINED. THUS, THE EQUIVALENCE RATIO CAN BE WRITTEN AS

$$\phi = \frac{\frac{m_F}{m_{O_2}}}{\left(\frac{m_F}{m_{O_2}}\right)_{st}} = \frac{\frac{N_F}{N_{O_2}}}{\left(\frac{N_F}{N_{O_2}}\right)_{st}} = \frac{X_F}{X_{O_2}} b = \frac{s Y_F}{Y_{O_2}}$$

$st$ = STOICHIOMETRIC CONDITIONS

$\left(\frac{m_F}{m_{O_2}}\right)_{st} = 1/s$ ; $\left(\frac{N_F}{N_{O_2}}\right)_{st} = 1/b$



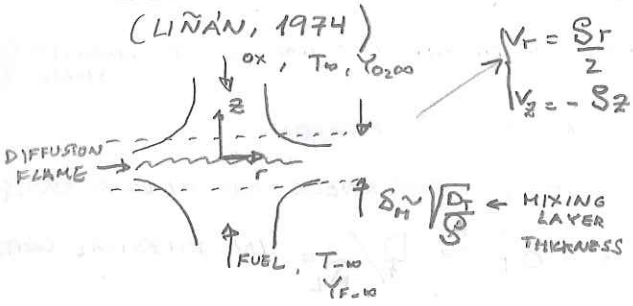

a: LEAN FLAMMABILITY LIMIT

b: RICH FLAMMABILITY LIMIT

THE MAXIMUM $S_L^0$ IS AT $\phi \gtrsim 1$ BECAUSE THE HEAT CAPACITY OF THE PRODUCTS ON THE RICH SIDE IS SLIGHTLY LOWER (IT CONTAINS MORE DIATOMIC GASES) THAN IN THE LEAN SIDE (IT CONTAINS MORE TRIATOMIC GASES)

## 2. ACTIVATION-ENERGY ANALYSES OF COUNTERFLOW DIFFUSION FLAMES

(LIÑÁN, 1974)




$S \sim \frac{U_j}{a}$ THE STRAIN RATE, WITH $U_j$ AND $a$ THE CHARACTERISTIC INJECTION VELOCITY AND ORIFICE DIAMETER

ASSUME A SINGLE STEP OF THE FORM

$$F + b O_2 \rightarrow P + q$$

$q$: CHEMICAL HEAT RELEASED PER UNIT MASS OF FUEL

WITH $s = \frac{b W_{O_2}}{W_F}$ AND

$\mathcal{S} = \frac{s Y_{F,\infty}}{Y_{O_2,\infty}}$ → MASS OF AIR ONE NEEDS TO MIX WITH THE UNIT MASS OF FUEL FEED STREAM TO GENERATE A STOICHIOMETRIC MIXTURE.

$\mathcal{S} \sim 10-15$ IN MOST COMBUSTION SYSTEMS

⇒ THAT $\mathcal{S}$ IS LARGE IMPLIES THAT THE FLAME NEEDS TO SIT DEEP WITHIN THE AIR STREAM (YET IN THE MIXING LAYER) TO SATISFY STOICHIOMETRY.

CONSERVATION EQUATIONS:

$$\nabla \cdot (\rho \underline{v}) = 0$$

$$\rho \underline{v} \cdot \nabla Y_F = \nabla \cdot (\rho D_F \nabla Y_F) - W_F \dot{\omega}$$

$$\rho \underline{v} \cdot \nabla Y_{O_2} = \nabla \cdot (\rho D_{O_2} \nabla Y_{O_2}) - b W_{O_2} \dot{\omega}$$

$$\rho c_p \underline{v} \cdot \nabla T = \nabla \cdot (\lambda \nabla T) + W_F q \dot{\omega}$$

- WITH $\dot{\omega} = A [F][O_2] e^{-\frac{E_a}{R^0 T}}$ ; $\left[\frac{m^3}{mol\,s}\right]$ THE CHEMICAL RATE
- ASSUME b) CONSTANT TRANSPORT PROPERTIES
  ii) CONSTANT DENSITY ⇒ THERMODIFFUSIVE LIMIT.

DEFINING $z' = \frac{z}{\sqrt{D_f/S}}$, $\hat{Y}_F = \frac{Y_F}{Y_{F,\infty}/(1+s)}$, $\hat{Y}_{O_2} = \frac{Y_{O_2}}{s Y_{O_2,-\infty}/(1+s)}$, $T' = \frac{T}{\frac{q Y_{F,\infty}}{c_p (1+s)}}$, THEN THE CONSERVATION EQUATIONS BECOME:

$i = F, O_2$ (1) $\frac{1}{Le_i} \frac{d^2 \hat{Y}_i}{dz^2} + z \frac{d \hat{Y}_i}{dz} = D_a \hat{Y}_F \hat{Y}_{O_2} e^{-\frac{T_a}{T}}$

DROPPED TILDES HERE

(2) $\frac{d^2 T}{dz^2} + z \frac{dT}{dz} = -D_a \hat{Y}_F \hat{Y}_{O_2} e^{-\frac{T_a}{T}}$

SUBJECT TO $\hat{Y}_{O_2} \rightarrow \frac{1+s}{s}$, $\hat{Y}_F \rightarrow 0$, AND $T \rightarrow T_\infty$ AT $z \rightarrow +\infty$,

AND $\hat{Y}_{O_2} \rightarrow 0$, $\hat{Y}_F \rightarrow 1+s$, $T \rightarrow T_{-\infty}$ AT $z \rightarrow -\infty$.

IN THIS FORMULATION, $T_a = \dfrac{E_a/R}{\dfrac{q\,Y_{F,\infty}}{c_p(1+s)}}$ IS THE DIMENSIONLESS ACTIVATION ENERGY,

NOTICE THAT $Y_{O_2,st} = \dfrac{s\,Y_{O_2,\infty}}{1+s}$.

AND $\boxed{D_a = \dfrac{s B\, Y_{O_2,\infty}}{(1+s)\,\rho}}$ IS THE PSEUDO-COLLISION DAMKÖHLER NUMBER, WHERE $B = \dfrac{\beta A}{W_{O_2}}$

IS A PSEUDO-COLLISION FREQUENCY [UNITS $\left(\frac{1}{s}\right)$] OF THE OVERALL STEP. THE PARAMETER $D_a$ IS THE RATIO OF THE FLOW TIME $t_r \sim 1/\rho$ TO THE COLLISION TIME $t_{COLL} \sim \left(\dfrac{B\,Y_{O_2,\infty}}{(1+s)}\right)^{-1}$.

ASSUME FURTHER THAT $Le_F = Le_{O_2} = 1 \Rightarrow$ A CONSERVED SCALAR $Z$, THE MIXTURE FRACTION, CAN BE THEN DEFINED AS $Z = \dfrac{s\,Y_F - Y_{O_2} + Y_{O_2,\infty}}{s\,Y_{F,\infty} + Y_{O_2,\infty}}$, OR EQUIVALENTLY,

$$Z = \frac{1}{1+s}\left\{ s\left(\frac{\hat{Y}_F - \hat{Y}_{O_2}}{1+s}\right) + 1 \right\}$$ IN NORMALIZED MASS FRACTIONS

$\rightarrow Z_{st} = \dfrac{1}{1+s}$ STOICHIOMETRIC MIXTURE FRACTION

- IN THE $O_2$ STREAM: $\hat{Y}_F = 0$, $\hat{Y}_{O_2} = \dfrac{1+s}{s} \Rightarrow Z = 0$
- IN THE F STREAM: $\hat{Y}_{O_2} = 0$, $\hat{Y}_F = 1+s \Rightarrow Z = 1$

(USING THIS AND COMBINING EQUATIONS (1) FOR F AND $O_2$ LEADS TO THE PROBLEM

$$\frac{d^2 Z}{dz^2} + 2\frac{dZ}{dz} = 0 \qquad \begin{cases} z \to +\infty, & Z \to 0 \\ z \to -\infty, & Z \to 1 \end{cases}$$

THE SOLUTION TO THIS EQUATION IS $Z = \dfrac{1}{2}\,\mathrm{erfc}\left(\dfrac{z}{\sqrt{2}}\right)$, WITH $\mathrm{erfc}(\cdot) = \dfrac{2}{\sqrt{\pi}}\displaystyle\int_0^{+\infty} e^{-t^2}\,dt$

A ISCALAR $\chi = D_T\left(\dfrac{dZ}{dz}\right)^2$ IS DEFINED AS THE SCALAR DISSIPATION RATE $\left(\text{UNITS } \frac{1}{s}\right)$, WHICH REPRESENTS A CHARACTERISTIC DIFFUSION TIME. IN UNITS OF $\frac{D_T}{}$, THE DIMENSIONLESS SCALAR DISSIPATION RATE BECOMES $\tilde{\chi} = \left(\dfrac{dZ}{dz}\right)^2 = \dfrac{1}{2\pi}\,e^{-z^2\delta_M^2}$, SO THAT

$$\tilde{\chi} = \frac{1}{2\pi}\,e^{-\left(\sqrt{2}\,\mathrm{erfc}^{-1}(2Z)\right)^2}$$

WHEN $s \gg 1$, $\chi_\rho \ll \chi_{MAX} \sim \rho$

NOTE THAT $\chi$ IS MAXIMUM AT THE STAGNATION PLANE, $\chi_{MAX} = \dfrac{\rho}{2\pi} \Rightarrow$ INDEPENDENT OF $D_T$

NOTE THAT, IN THE $Z$ VARIABLE, THE OPERATOR $\dfrac{d^2}{dz^2} + 2\dfrac{d}{dz}$ BECOMES

$$\frac{d^2}{dz^2} + 2\frac{d}{dz} = \left(\frac{d^2 Z}{dz} + 2\frac{dZ}{dz}\right)\frac{d}{dz} + \left(\frac{dZ}{dz}\right)^2\frac{d^2}{dZ^2} = \tilde{\chi}\frac{d^2}{dZ^2}, \quad \text{AND THEREFORE}$$

($\frac{d^2 Z}{dz} + 2\frac{dZ}{dz} = 0$)

$\tilde{\chi}^{-1}$ BEHAVES AS AN INTEGRATING FACTOR OF THE CONSERVATION EQUATIONS.

DISSIPATION IS INDEPENDENT OF MOLECULAR DIFFUSIVITY.

A SECOND CONSERVED SCALAR $H$, THE EXCESS ENTHALPY, CAN BE DEFINED AS $H = \dfrac{\hat{Y}_F + s\hat{Y}_{O_2}}{1+s} - 1 + T - T_\infty$, WITH

- $H = 0$ IN THE OXIDIZER STREAM,
- $H = T_{-\infty} - T_\infty$ IN THE FUEL STREAM.

USING THIS AND COMBINING EQUATIONS (1) AND (2) ONE ARRIVES TO THE PROBLEM $\dfrac{d^2 H}{dZ^2} = 0$, WITH $H = 0$ AT $Z = 0$ AND $H = T_{-\infty} - T_b = -\beta_T/Z_{st}$ AT $Z = 1 \Rightarrow H = -\beta_T Z/Z_{st}$. THE DEFINITIONS OF $H, Z, \chi$ REDUCE THE PROBLEM (1) AND (2) INTEGRATING:

(3)

$$\left.\begin{aligned} \tilde{\chi}(Z)\frac{d^2 T}{dZ^2} &= -D_a\,Y_F\,Y_{O_2}\,e^{-\frac{T_a}{T}} \\ \hat{Y}_F &= (1-\beta_T)\,Z/Z_{st} + T_\infty - T \\ \hat{Y}_{O_2} &= \frac{1+s}{s} - \left[\beta_T + 1/s\right]Z/Z_{st} + T_\infty - T \end{aligned}\right\} \quad \text{SUBJECT TO } T \to T_\infty,\ Z \to 1 \text{ AND } T \to T_\infty,\ Z \to 0$$

THE ORIGINAL FLAMELET PROBLEM (LIÑÁN, 1974)

WHEN LIÑÁN ARRIVED TO THE PROBLEM (2), HE IDENTIFIED 4 DISTINGUISHED BURNING REGIMES: i) AN IGNITION REGIME, IN WHICH IGNITION IS PRODUCED BY AN INCREASE IN THE DAMKÖHLER NUMBER SUFFICIENT TO CAUSE TEMPERATURE VARIATIONS OF ORDER $1/\beta$, WITH $\beta = \frac{T_a}{T_\infty^2} \gg 1$ (NON DIMENSIONAL TEMPERATURES) THE ZEL'DOVICH NUMBER IN THE IGNITION REGIME, (REMINDER: $\dot{\omega} \sim e^{-\frac{T_a}{T_0}} e^{-\beta\left(\frac{T-T_0}{T/T_0}\right)}$ → SMALL TEMPERATURE VARIATIONS LEAD TO ORDER-UNITY VARIATIONS OF THE REACTION RATE AT $\beta \gg 1$ (AEA)), IN AN INITIALLY FROZEN MIXTURE OF FUEL AND OXIDIZER; ii) A PARTIAL-BURNING REGIME, IN WHICH $O(1)$ LEAKAGE OF FUEL AND OXIDIZER OCCURS THROUGH THE FLAME (UNSTABLE REGIME); iii) A PREMIXED-FLAME REGIME, IN WHICH EXTINCTION OCCURS WITH $O(1)$ LEAKAGE OF ONE OF THE REACTANTS (→ PREFERENTIALLY FUEL) THROUGH THE FLAME RESEMBLING AN INNER PREMIXED-FLAME STRUCTURE; AND iv) A DIFFUSION-FLAME REGIME, IN WHICH NO REACTANT LEAKAGE OCCURS IN THE FIRST APPROXIMATION ($\hat{\mu}$.e THE FAST CHEMISTRY OR BURKE-SCHUMANN LIMIT), AND EXTINCTION OCCURS WITH $O(1/\beta)$ LEAKAGE THROUGH THE FLAME, WITH $\beta = \frac{T_a}{T_f^2} \gg 1$

$\chi_f = \chi|_{z_{st}} \rightarrow t_d \sim \frac{1}{\chi_f}$

DEFINING $\Delta = \frac{t_d}{t_c} = \frac{\text{DIFFUSION TIME THROUGH THE FLAME}}{\text{LOCAL CHEMICAL TIME}} =$ REDUCED DAMKÖHLER NUMBER

THEN A SOLUTION OF (3) IN THE FORM OF AN $S$-CURVE CAN BE OBTAINED.

* THE BURKE-SCHUMANN LIMIT:

A DIFFUSION-CONTROLLED COMBUSTION REGIME EXISTS FOR LARGE DAMKÖHLER NUMBERS, IN WHICH THE TEMPERATURE AND COMPOSITION FIELDS DO NOT DEPEND ON THE CHEMICAL KINETICS IN THE FIRST APPROXIMATION. IN THIS REGIME, THE CHEMICAL TIME $t_c \sim \left(\frac{B S Y_{O_2,\infty}}{1+S}\right)^{-1} e^{-\frac{T_a}{T_f}}$ IS MUCH SHORTER THAN THE DIFFUSION TIME $t_d \sim 1/\chi_f$, SO THAT $\Delta = \frac{t_d}{t_c} \gg 1$. THE FLOW REMAINS IN CHEMICAL EQUILIBRIUM ON BOTH SIDES OF A THIN REACTION SHEET OF INFINITESIMAL THICKNESS, AND NO REACTANT LEAKAGE OCCURS IN A FIRST APPROXIMATION. IN THIS FORMULATION, $T_f$ IS THE EQUILIBRIUM FLAME TEMPERATURE IN THE BURKE SCHUMANN LIMIT, WHICH IS CLOSE TO THE ADIABATIC FLAME TEMPERATURE.

TO LEADING ORDER IN $1/\beta$, $\hat{Y}_F \hat{Y}_{O_2} = 0$ AT THE THIN FLAME, WITH $\hat{Y}_F = 0$ FOR $Z < Z_{st}$ AND $\hat{Y}_{O_2} = 0$ FOR $Z > Z_{st}$, WITH $\dot{\omega}$ APPROXIMATED AS A DELTA-DIRAC FUNCTION. IN THIS LIMIT, THE SOLUTION TO (3) BECOMES: (BURKE-SCHUMANN TEMP.) $T_f = T_\infty + 1 - \beta_T$

(4)

IN THE FUEL REGION $Z_{st} < Z < 1$:
$$T = T_\infty + 1 + \frac{1}{S} - \left(\frac{1}{S} + \beta_T\right) Z/Z_{st}$$
$$\hat{Y}_F = \left(\frac{1+S}{S}\right)\left(\frac{Z}{Z_{st}} - 1\right), \quad \hat{Y}_{O_2} = 0$$

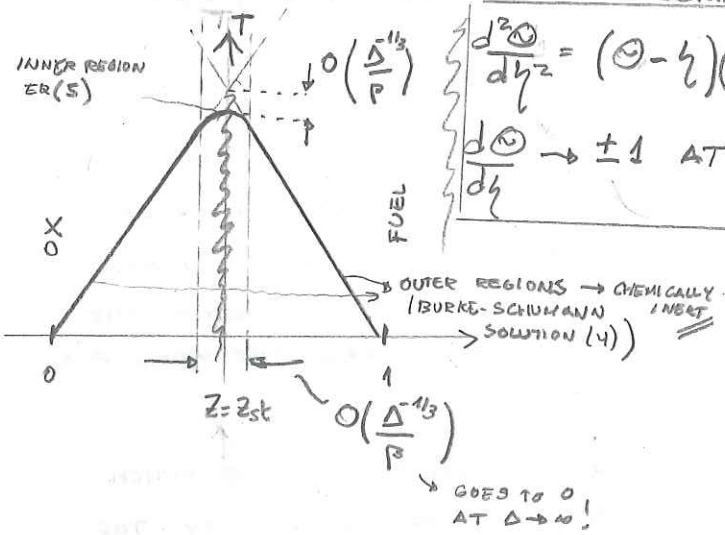
(EQUATING BOTH TEMPERATURES AT $Z = Z_{st}$)

IN THE OXIDIZER REGION $0 < Z < Z_{st}$:
$$T = T_\infty + (1 - \beta_T) Z/Z_{st}$$
$$\hat{Y}_{O_2} = \left(\frac{1+S}{S}\right)\left(1 - \frac{Z}{Z_{st}}\right), \quad \hat{Y}_F = 0$$

## * NEAR-EXTINCTION REGION (DIFFUSION-FLAME REGIME)

NON-EQUILIBRIUM EFFECTS ASSOCIATED WITH FINITE-RATE CHEMISTRY AND FINITE DAMKÖHLER NUMBERS LEAD TO EXTINCTION WHEN THE DIFFUSION TIME THROUGH THE MIXING-LAYER PROBLEM BECOMES OF THE SAME ORDER AS THE CHEMICAL TIME.

TO $O(1/\beta)$, BOTH REACTANTS DIFFUSE INTO A FLAME REGION OF THICKNESS $O\left(\Delta^{1/3}/\beta\right)$, IN WHICH TEMPERATURE VARIATIONS ARE OF ORDER $O\left(\frac{\Delta^{-1/3}}{\beta}\right)$ WITH RESPECT TO $T_f$. INTRODUCING THE ASYMPTOTIC EXPANSION $T = T_f - \Delta^{-1/3}\left[\frac{\Theta}{\beta} + \frac{\gamma\eta}{\beta} + O\left(\frac{1}{\beta^2}\right)\right]$, (WITH $\beta = \frac{T_a}{T_f^2} \gg 1$), IN EQ (3). THE FOLLOWING PROBLEM IS OBTAINED:




$$\frac{d^2\Theta}{d\eta^2} = (\Theta - \eta)(\Theta + \eta)\, e^{-\Delta^{-1/3}(\Theta + \gamma\eta)} \qquad (5)$$

$$\frac{d\Theta}{d\eta} \to \pm 1 \quad \text{AT} \quad \eta \to \pm\infty$$

DIFFUSION-FLAME INNER-REGION STRUCTURE (LIÑÁN, 1974)

WITH $\gamma$ A PARAMETER THAT DEPENDS ON THE NET ENTHALPY GRADIENT,

$$\eta = \frac{\Delta_0^{1/3}(1+s)}{2s}\beta\left(Z - Z_{st}\right)$$ AN INNER CORDINATE

$\delta_f \sim \frac{\Delta_0^{1/3}}{\beta}\delta_D$ DIFFUSION-FLAME THICKNESS

AND $\Delta_0 = \frac{4 Z_{st}^2 D_{a_0} e^{-\frac{T_a}{T_f}} s^2}{\tilde{\chi}_f (1+s)^2 \beta^3} = \frac{t_d}{t_c}$ THE REDUCED DAMKÖHLER NUMBER.

$t_d$: DIFFUSION TIME; $t_c$: CHEMICAL TIME.

AT EXTINCTION, $\Delta_0 \sim O(1)$, AND ANALYSIS OF (5) SHOWS THAT THERE IS A CRITICAL POINT $\Delta_0 = \Delta_{0E}$ REPRESENTATIVE OF EXTINCTION BELOW WHICH NO SOLUTION TO (5) EXISTS. IN PARTICULAR,

$$\Delta_{0E} \simeq e^1\left[(1-|\gamma|) - (1-|\gamma|)^2 + 0.26(1-|\gamma|)^3 + 0.155(1-|\gamma|)^4\right]$$

IS THE EXTINCTION DAMKÖHLER NUMBER, SO THAT,

$$\Delta_{0E} = \frac{4 Z_{st}^2 D_{a_E} e^{-\frac{T_a}{T_f}} s^2}{\tilde{\chi}_q (1+s)^2 \beta^3}$$ AND $\delta_f \sim \delta_M/\beta$ ARE VERIFIED AT EXTINCTION,

WITH $\hat{Y}_O \sim O(1/\beta)$, $\hat{Y}_F \sim O(1/\beta)$ LEAKAGE THROUGH THE FLAME.

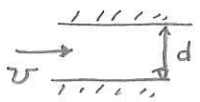
THE ANALYSIS ABOVE WAS THE FUNDAMENTAL BASIS FOR THE CONSTRUCTION OF EARLY FLAMELET MODELS (SEE, FOR INSTANCE: PETERS N., COMB. SCI. TECH 30: 1-6, 1983)

### REVIEW OF TURBULENT FLOWS

- CHARACTERISTICS OF TURBULENCE:
  - i) IRREGULARITY (RANDOMNESS) ⇒ NEED OF STATISTICAL APPROACH
  - ii) INCREASED DIFFUSIVITY ⇒ INCREASED MIXING AND HEAT RELEASE
  - iii) $Re \gg 1$ ⇒ NON-LINEARITY
  - iv) THREE-DIMENSIONAL VORTICITY FLUCTUATIONS: THE RANDOM FLUCTUATIONS OF $\vec{\omega}$, WHICH CHARACTERIZE TURBULENCE, COULD NOT MANTAIN THEMSELVES IF THE VELOCITY FLUCTUATIONS WERE 2D.
  - v) DISSIPATION: TURBULENCE IS DISSIPATIVE
  - vi) CONTINUUM: TURBULENCE IS CONTINUUM EVEN AT THE SMALLEST SCALES, WHICH ARE MUCH LARGER THAN THE MEAN FREE PATH

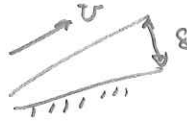
- STATISTICAL METHODS OF ANALYSIS TYPICALLY LEAD TO THE "CLOSURE PROBLEM", IN THAT MORE UNKNOWNS THAN EQUATIONS APPEAR. A USUAL POSTULATE IS TO ASSUME A RELATION BETWEEN STRESS AND STRAIN THAT INVOLVES A TURBULENCE-GENERATED VISCOSITY $\nu_T$. → SEE FIG 14

- TURBULENCE IS GENERATED BY INSTABILITIES AT HIGH REYNOLDS NUMBERS

Ex 

CHANNEL FLOW

$Re_d = \frac{Ud}{\nu} \gtrsim 2000$



BOUNDARY LAYER

$Re_{\delta''} = \frac{U\delta''}{\nu} \gtrsim 600$

- TURBULENCE CAN BE SUPPRESED BY MECHANISMS THAT CONSUME TURBULENT KINETIC ENERGY, AT LARGE Re, THE NON-LINEAR TERMS IN THE N-S EQUATIONS GENERATE MOTION AT SMALL SCALES ENOUGH TO BE AFFECTED BY VISCOSITY. AS SOON AS THE SCALE OF THE FLOW FIELD BECOMES SO LARGE THAT VISCOSITY EFFECTS COULD NOT BE NEGLECTED, THE NONLINEARITIES GENERATE SMALL-SIZED MOTIONS, IN SUCH A WAY THAT VISCOSITY EFFECTS (DISSIPATION) ARE KEPT AT A FINITE LEVEL → SEE FIG 14

- IN TURBULENT FLOWS A WIDE RANGE OF SCALES EXISTS, BOUNDED FROM ABOVE BY THE DIMENSIONS OR TIME SCALES OF THE GEOMETRY OR BOUNDARY CONDITIONS, AND FROM BELOW BY THE SCALES DOMINATED BY MOLECULAR DIFFUSION. IN GENERAL, THE SCALES DOMINATED BY MOLECULAR DIFFUSION HAVE THE FASTEST TURNOVER TIMES, SO ONE MAY ENVISION SOME DEGREE, IF NOT COMPLETE, OF STATISTICAL INDEPENDENCE IN THESE SCALES FROM THE MEAN FLOW.

KOLMOGOROV UNIVERSAL EQUILIBRIUM THEORY:

SINCE THE SMALL SCALES TURN FASTER, THEY SHOULD DEPEND ONLY ON THE RATE AT WHICH THEY ARE SUPPLIED WITH ENERGY FROM THE LARGER SCALES AND ON KINEMATIC VISCOSITY. THE RATE OF ENERGY SUPPLY SHOULD BE EQUAL TO THE RATE OF DISSIPATION (DYNAMICAL EQ.), BECAUSE THE NET RATE OF CHANGE OF SMALL-SCALE ENERGY IS RELATED TO THE TIME SCALE OF THE FLOW, AND THE LATTER IS LONG.

INTRODUCING THE DISSIPATION RATE $\varepsilon \sim u'^3/\ell = \frac{u'^2}{\ell/u'} \sim \frac{u'^2}{T}$ $\left[\frac{m^2}{s^3}\right]$ AT $Re_\ell \gg 1$

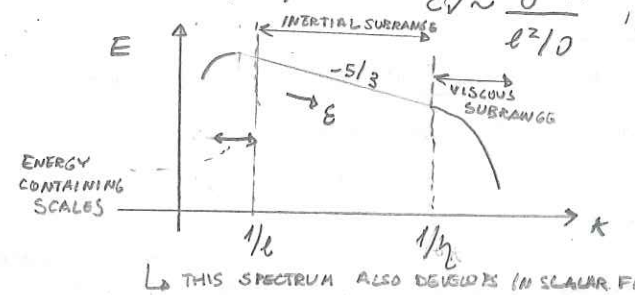
THE KOLMOGOROV MICROSCALES (OR INNER SCALES) ARE

$$l_k = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}, \quad \tau = \left(\frac{\nu}{\varepsilon}\right)^{1/2}, \quad v = (\nu\varepsilon)^{1/4}, \text{ WITH } \frac{l_k v}{\nu} \sim 1$$

WITH $\frac{l_k}{\ell} \sim Re_\ell^{-3/4}$, $\frac{\tau}{T} \sim Re_\ell^{-1/2}$, $\frac{v}{u'} \sim Re_\ell^{-1/4}$, WITH $Re_\ell = \frac{u'\ell}{\nu} \gg 1$

IN THIS FORMULATION, $u'$ IS THE CHARACTERISTIC LARGE-EDDY TURNOVER VELOCITY, $T$ IS THE CHARACTERISTIC INTEGRAL TIMESCALE, AND $\ell \approx T/u'$ IS THE CHARACTERISTIC INTEGRAL LENGTH. NOTE THAT $\varepsilon$ DOES NOT DEPEND ON $\nu$, AND THAT TURBULENT DISSIPATION ACTS IN A MUCH FASTER TIME SCALE THAN THE LARGE-SCALE VISCOUS DISSIPATION ($\varepsilon_\nu$): $\varepsilon_\nu \sim \frac{u'^2}{\ell^2/\nu}$, $\frac{\varepsilon_\nu}{\varepsilon} \sim Re_\ell^{-1} \ll 1$, AND THAT $\varepsilon \sim \frac{u'^3}{\ell} \sim \frac{\nu^3}{\eta}$.

$T \sim \frac{k}{\varepsilon}$, WITH $k \sim \frac{3u'^2}{2}$ THE TURBULENT KINETIC ENERGY




↳ THIS SPECTRUM ALSO DEVELOPS IN SCALAR FIELDS

- IF $k$ IS THE WAVENUMBER, $k \sim 1/\ell$, THEN THE KINETIC ENERGY OF AN EDDY OF SIZE $\ell_m$ IS $v_m^2 \sim \varepsilon^{2/3} k^{-2/3}$;

- THE VORTICITY IN THE MICROSCALE IS $Re^{1/2}$ LARGER THAN THAT OF LARGE-SCALE MOTIONS

| LARGE SCALES | $\xrightarrow{\varepsilon}$ | SMALL SCALES |
|---|---|---|
| $u', \ell, T$ | | $\ell_K, \tau_K, \nu$ |
| - LONG TIMESCALES $T$ BUT $T \ll \ell^2/\nu$ | | - SHORT TIMESCALES $\tau \ll T$ |
| - LARGE VELOCITIES $u'$ | | - SMALL VELOCITIES $\nu$ |
| - SMALL VORTICITY $\sim 1/T$ | | - LARGE VORTICITY $\sim 1/\tau_K$ |
| - SMALL STRAIN RATE | | - LARGE STRAIN RATE |
| ⇓ KINETIC ENERGY PEAKS HERE | | ⇓ DISSIPATION, ENSTROPHY AND STRAIN RATE PEAK HERE |

NOTICE THAT, IF $\lambda_a \sim \nu/a$ IS THE MEAN FREE PATH, WITH $a$ THE SPEED OF THE SOUND WAVES, THEN

$\frac{\lambda_a}{\eta} \sim \frac{M}{Re_\ell^{1/4}}$ IS TYPICALLY A SMALL NUMBER

AND $\frac{\tau}{\lambda_a/a} \sim \frac{Re_\ell^{1/2}}{M^2}$ IS TYPICALLY A LARGE NUMBER

⇒ THE SMALLEST EDDIES LIVE IN A CONTINUUM AND THE GAS IS IN STATISTICAL EQUILIBRIUM

## STATISTICAL DESCRIPTION OF TURBULENT FLOWS

CONSIDER $U$ = STOCHASTIC VARIABLE AND $\mathcal{U}$ = SAMPLE SPACE OF $U$ (ALL REALIZATIONS). THE DISTRIBUTION FUNCTION $F_U(\mathcal{U}) = P(U < \mathcal{U})$ IS DEFINED AS THE PROBABILITY OF $U < \mathcal{U}$, WITH $P(\mathcal{U}_- < U < \mathcal{U}_+) = F_U(\mathcal{U}_+) - F_U(\mathcal{U}_-)$ THE PROBABILITY OF FINDING $U$ IN THE INTERVAL $(\mathcal{U}_-, \mathcal{U}_+)$. THE PROBABILITY-DENSITY FUNCTION IS $P_U(\mathcal{U}) = \frac{dF_U(\mathcal{U})}{d\mathcal{U}}$, WITH $P_U(\mathcal{U})\,d\mathcal{U} = P(\mathcal{U} < U < \mathcal{U} + d\mathcal{U})$, USUALLY SUBJECT TO THE NORMALIZATION CONDITION $\int_{-\infty}^{+\infty} P_U(\mathcal{U})\,d\mathcal{U} = 1$. IN GENERAL, $P_U = P_U(\mathcal{U}; \underline{x}, t)$, WITH $P_U = P_U(\mathcal{U}; \underline{x})$ ONLY FOR STATIONARY TURBULENCE, AND $P_U = P_U(\mathcal{U}; t)$ FOR HOMOGENEOUS TURBULENCE.

- MOMENTS: $\overline{U^m(\underline{x},t)} = \int_{-\infty}^{+\infty} \mathcal{U}^m P(\mathcal{U}; \underline{x}, t)\,d\mathcal{U}$, WITH $\overline{U(\underline{x},t)} = \int_{-\infty}^{+\infty} \mathcal{U} P(\mathcal{U}; \underline{x}, t)\,d\mathcal{U}$ THE FIRST MOMENT OR EXPECTATION, AND $\overline{\left[U(\underline{x},t) - \overline{U(\underline{x},t)}\right]^2} = \int_{-\infty}^{+\infty} (\mathcal{U} - \bar{U})^2 P(\mathcal{U}; \underline{x}, t)\,d\mathcal{U} = \overline{u'^2} = \overline{U^2} - \bar{U}^2$ THE SECOND MOMENT OR VARIANCE, WHERE $U$ HAS BEEN SPLIT IN A MEAN AND FLUCTUATIONS: $U = \bar{U} + u'$, WITH $(u'^2)^{1/2}$ THE RMS VELOCITY
  - THE VARIANCE IS THE MEAN OF THE FLUCTUATIONS SQUARED
- JOINT PDF: $P(\mathcal{U}, \mathcal{V}; \underline{x}, t)$
- MARGINAL PDF: $P(\mathcal{U}) = \int_{-\infty}^{+\infty} P(\mathcal{U}, \mathcal{V})\,d\mathcal{V}$
- CORRELATION BETWEEN $u'$ AND $v'$: $\overline{u'v'} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (\mathcal{U} - \bar{U})(\mathcal{V} - \bar{V}) P(\mathcal{U}, \mathcal{V})\,d\mathcal{U}\,d\mathcal{V} = \overline{UV} - \bar{U}\bar{V}$

AND CORRELATION COEFFICIENT $C = \frac{\overline{u'v'}}{(\overline{u'^2}\,\overline{v'^2})^{1/2}}$

- BAYES THEOREM: A JOINT PDF OF TWO INDEPENDENT VARIABLES CAN BE WRITTEN AS A PRODUCT OF A CONDITIONAL PDF OF ONE VARIABLE TIMES THE MARGINAL PDF OF THE OTHER: $P(\mathcal{U}, \mathcal{V}; \underline{x}, t) = P(\mathcal{U}|\mathcal{V}; \underline{x}, t)\,P(\mathcal{V}; \underline{x}, t)$

IF $U$ AND $V$ ARE NOT CORRELATED, THEY ARE SAID TO BE STATISCALLY INDEPENDENT, AND $C = 0 \rightarrow P(\mathcal{U}, \mathcal{V}; \underline{x}, t) = P(\mathcal{U}; \underline{x}, t)\,P(\mathcal{V}; \underline{x}, t)$

⇒ TURBULENCE IS CHARACTERIZED BY STRONG CORRELATIONS OF THE VELOCITY FLUCTUATIONS $\overline{u'v'}$, BY WHICH TURBULENCE EXCHANGES MOMENTUM WITH THE MEAN FLOW.

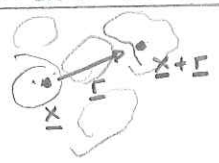
- CONDITIONAL MOMENTS: $\langle U|V\rangle = \int_{-\infty}^{+\infty} \mathcal{U} P(\mathcal{U}|\mathcal{V})\,d\mathcal{U}$ CONDITIONAL MEAN.

### AVERAGING

- REYNOLDS AVERAGING: $U = \bar{U} + u'$, WITH
  - $\bar{U} = \lim_{T\to\infty} \frac{1}{T}\int_{t_0}^{t_0+T} U\,dt$ TIME AVERAGING FOR STATISTICALLY STEADY FLOWS.
  - $\bar{U} = \lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} U_n$ (OVER $N$ REPETITIONS)
- FAVRE AVERAGING: $U = \tilde{U} + u''$, WITH $\tilde{U}$ A DENSITY-WEIGHTED AVERAGE SUCH THAT $\overline{\rho u''} = 0$, OR EQUIVALENTLY, $\overline{\rho U} = \overline{\rho}\tilde{U} + \overline{\rho u''}^{\,0} \rightarrow \boxed{\tilde{U} = \overline{\rho U}/\overline{\rho}}$ → FOR VARIABLE-DENSITY FLOWS (COMBUSTION)

$\overline{(U-\bar{U})^2} = \overline{U^2 - 2U\bar{U} + \bar{U}^2} = \overline{U^2} - \bar{U}^2$

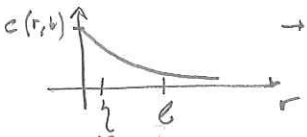
- INTEGRAL LENGTH SCALE: (VELOCITIES) = CONSIDER THE 2-POINT VELOCITY CORRELATIONS:




$$R(\underline{x},\underline{r},t) = \overline{\underline{u}'(\underline{x},t)\,\underline{u}'(\underline{x}+\underline{r},t)}$$

FOR HOMOGENEOUS ISOTROPIC TURBULENCE R IS INDEPENDENT OF $\underline{x}$ AND $\underline{r}$ IS INDEPENDENT OF THE ORIENTATION. THE CORRELATION COEFFICIENT BECOMES

$$c(r,t) = \frac{R(r,t)}{u'^2(t)}$$




→ SMALL DISTANCES → HIGH CORRELATION

⇒ INTEGRAL LENGTH SCALE $\ell = \int_0^\infty c\,dr$ ⇒ THE KINETIC ENERGY LIVES IN THESE SCALES

IN GENERAL, R IS A TENSOR, $R_{ij}(\underline{x},\underline{r},t) = u_i'(\underline{x},t)\,u_j'(\underline{x}+\underline{r},t)$, WHICH YIELDS THE SPECTRUM TENSOR $\phi_{ij}(\underline{\kappa}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{+\infty} e^{-i\underline{\kappa}\cdot\underline{r}} R_{ij}(\underline{r})\,d\underline{r}$, WITH $\underline{\kappa}$ THE WAVENUMBER VECTOR.

THE TRACE OF THE SPECTRUM TENSOR IS THE KINETIC ENERGY AT A GIVEN WAVENUMBER, WITH $R_{ii}(0) = \overline{u_i' u_i'} = 2k$. INTEGRAL LENGTH SCALES CAN BE CALCULATED FROM THE CORRELATION TENSOR, SUCH AS THE LONGITUDINAL INTEGRAL LENGTH SCALE $L_{11} = \frac{1}{R_{11}(\underline{x},0,t)}\int_0^\infty R_{11}(\underline{r},\underline{x},t)\,d\underline{r}$

THE ENERGY-SPECTRUM FUNCTION IS OBTAINED BY INTEGRATING $\phi_{ij}$ OVER A SPHERE $S(|\underline{\kappa}|)$ IN WAVENUMBER SPACE, CENTERED AT THE ORIGIN, WITH RADIUS $|\underline{\kappa}| = \kappa$: $E(|\underline{\kappa}|) = \oint_S \frac{\phi_{ij}}{2}(\underline{\kappa})\,dS(|\kappa|)$

⇒ KINETIC ENERGY: $k = \int_0^\infty E(\kappa)\,d\kappa$

⇒ DISSIPATION: $\varepsilon = \int_0^\infty 2\nu\kappa^2 E(\kappa)\,d\kappa$

INTEGRAL LENGTH SCALE (OVERALL): $\ell = k^{3/2}/\varepsilon$

INTEGRAL TIME SCALE (OVERALL): $T \approx k/\varepsilon$

TAYLOR HYPOTHESIS! → VELOCITY SIGNAL FROM A MOVING PROBE AT SPEED $\bar{U}$, $u(t)$ MAY BE IDENTIFIED WITH $u(x/\bar{U})$ IF $\frac{u}{\bar{U}} \ll 1$. IT TENDS TO FAIL IN SHEAR FLOWS (POPE)

- REYNOLDS-AVERAGED N-S EQUATIONS ($\rho$ = CONST)

$\underline{U} = \underline{\bar{U}} + \underline{u}'$ ⇒ CONTINUITY: $\nabla\cdot\underline{\bar{U}} = 0$

⇒ MOMENTUM: $\underline{\bar{U}}\cdot\nabla\underline{\bar{U}} = -\nabla\cdot(\overline{\underline{u}'\underline{u}'}) - \frac{\nabla\bar{P}}{\rho} + \nu\nabla^2\underline{\bar{U}}$

$\overline{\underline{U}\underline{U}} = \overline{(\underline{\bar{U}}+\underline{u}')(\underline{\bar{U}}+\underline{u}')} = \underline{\bar{U}}\,\underline{\bar{U}} + \overline{\underline{\bar{U}}\,\underline{u}'} + \overline{\underline{u}'\,\underline{\bar{U}}} + \overline{\underline{u}'\underline{u}'}$

OR EQUIVALENTLY: $\rho\underline{\bar{U}}\cdot\nabla\underline{\bar{U}} = -\nabla\bar{P} + \nabla\cdot(\underbrace{\bar{\tau}' - \rho\overline{\underline{u}'\underline{u}'}}_{\text{MODIFIED STRESS}})$, WITH $-\rho\overline{\underline{u}'\underline{u}'}$ THE REYNOLDS STRESS (UNCLOSED)

⇒ SPECIES (NON REACTING): $\rho\underline{\bar{U}}\cdot\nabla\bar{Y} = -\nabla\cdot(\underbrace{\rho\underline{\bar{V}}\bar{Y} + \rho\overline{\underline{u}'Y'}}_{\text{MODIFIED FLUX}})$, WITH $-\rho\overline{u'Y'}$ THE TURBULENT SCALAR FLUX (UNCLOSED)

⇒ SPECIES (REACTING): $\rho\underline{\bar{U}}\cdot\nabla\bar{Y} = -\nabla\cdot(\rho\underline{\bar{V}}\bar{Y} + \rho\overline{\underline{u}'Y'}) + \dot{\bar{w}}$, WITH $\dot{\bar{w}}$ THE MEAN REACTION RATE (UNCLOSED)

- FAVRE-AVERAGED N-S EQUATIONS ($\rho$ ≠ CONST)

$U = \tilde{U} + U''$, WITH $\overline{\rho U''} = 0$. THEN $\overline{\rho U} = \overline{\rho(\tilde{U}+U'')} = \bar{\rho}\tilde{U} + \overline{\rho U''}^{\,0} \Rightarrow \tilde{U} = \frac{\overline{\rho U}}{\bar{\rho}}$.

NOTICE THAT $\overline{\rho\tilde{U}} = \bar{\rho}\tilde{U}$ BECAUSE $\tilde{U}$ IS ALREADY AVERAGED!

FOR ANY VARIABLE $\phi$: $\tilde{\phi} = \overline{\rho\phi}/\bar{\rho}$ IS THE FAVRE-MEAN.

FOR INSTANCE: $\overline{\rho UV} = \overline{\rho\tilde{U}\tilde{V}} + \overline{\rho\tilde{U}U''} + \overline{\rho\tilde{V}U''}^{\,0} + \overline{\rho U''V''} = \bar{\rho}\tilde{U}\tilde{V} + \overline{\rho U''V''} = \bar{\rho}\tilde{U}\tilde{V} + \bar{\rho}\,\widetilde{U''V''}$

WITH FAVRE AVERAGING: i) $\rho$-FLUCTUATIONS DON'T APPEAR IN THE FORMULATION.

ii) CROSS-CORRELATIONS SUCH AS $\overline{\rho'\phi'}$ DO NOT APPEAR IN THE FORMULATION.

BOTH i) AND ii) WOULD APPEAR IF REYNOLDS AVERAGING WAS APPLIED IN DENSITY-VARYING FLOWS:

Ex: $\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\underline{U}) = 0$

- WITH REYNOLDS AVERAGING: $\frac{\partial\bar{\rho}}{\partial t} + \nabla\cdot(\bar{\rho}\underline{\bar{U}}) = -\nabla\cdot(\overline{\rho'\underline{u}'})$ UNCLOSED!

- WITH FAVRE AVERAGING: $\frac{\partial\bar{\rho}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{U}) = 0$

THERE IS NO SIMPLE RELATION BETWEEN FAVRE AND REYNOLDS AVERAGES. A RELATION BETWEEN THESE TWO QUANTITIES REQUIRES KNOWLEDGE OR MODELING OF DENSITY FLUCTUATION CORRELATIONS SINCE $\overline{\rho\tilde{\phi}} = \overline{\rho\phi} = \bar{\rho}\bar{\phi} + \overline{\rho'\phi'}$ FOR ANY $\phi$. $\Rightarrow$ CAUTION AT COMPARING NUMERICAL SIMULATIONS ($\tilde{\phi}$) WITH EXPERIMENTS (TYPICALLY $\bar{\phi}$)

THE FAVRE-AVERAGED N-S EQUATIONS BECOME:

($\Rightarrow$ PROCEDURE: APPLY OVERBAR $(\bar{-})$ TO EQUATIONS AND THEN EXPAND $u$, $Y$ AND $h$ IN FAVRE AVERAGE + FLUCTUATION!)

- CONTINUITY: $\frac{\partial \bar{\rho}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}) = 0$

- MOMENTUM: $\frac{\partial \bar{\rho}\tilde{\underline{u}}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{\underline{u}}) = -\nabla\bar{P} + \nabla\cdot\bar{\underline{\tau}}' - \nabla\cdot(\bar{\rho}\widetilde{u''v''})$

$\Rightarrow$ WHEN $\frac{\partial}{\partial t}$ IS RETAINED, IT IS IMPLIED THE CALCULATION IS MADE FOR ENSEMBLE AVERAGES.

- SPECIES: $\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{Y}_i) = -\nabla\cdot(\overline{\underline{V}_i Y_i}) - \nabla\cdot(\bar{\rho}\widetilde{u''Y_i''}) + \bar{\dot{w}}_i$ FOR $i = 1, \dots N$

- SENSIBLE ENTHALPY: $\frac{\partial}{\partial t}(\bar{\rho}\tilde{h}_s) + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{h}_s) = \overline{\frac{Dp}{Dt}} + \overline{\bar{\tau}:\nabla\underline{u}} + \nabla\cdot(\overline{\kappa\nabla T}) - \nabla\cdot(\bar{\rho}\widetilde{\underline{u}''h_s''})$

$$- \nabla\cdot\left(\sum_{i=1}^{N}\overline{\rho h_{s_i} Y_i \underline{V}_i}\right) - \sum_{i=1}^{N} h_i^0 \bar{\dot{w}}_i \,, \quad \text{WITH } \overline{\frac{Dp}{Dt}} = \frac{\partial\bar{p}}{\partial t} + \tilde{\underline{u}}\cdot\nabla\bar{p} + \overline{\underline{u}''\cdot\nabla p}$$

WHERE EFFECTS OF BODY FORCES AND RADIATION HAVE BEEN NEGLECTED. THE UNCLOSED TERMS IN THE EQUATIONS ABOVE ARE:

i) THE SPECIES AND ENTHALPY TURBULENT FLUXES: GENERALLY CLOSED USING A CLASSICAL GRADIENT ASSUMPTION: $\bar{\rho}\widetilde{\underline{u}''Y_i''} = -\frac{\mu_t}{Sc_t}\nabla\tilde{Y}_i$, AND $\bar{\rho}\widetilde{\underline{u}''h_s''} = -\frac{\mu_t}{Pr_t}\nabla\tilde{h}_s$,

WITH $\mu_t$ A TURBULENT (EDDY) VISCOSITY, WHICH NEEDS MODELLING, AND $Sc_t$ AND $Pr_t$ THE TURBULENT SCHMIDT AND TURBULENT PRANDTL NUMBERS, RESPECTIVELY, WHICH NEED CALIBRATION.

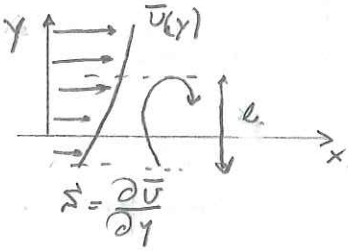
ii) PRESSURE-VELOCITY CORRELATION: $\overline{\underline{u}''\cdot\nabla P}$, WHICH IS NEGLECTED IN MOST RANS CODES

iii) MOLECULAR DIFFUSION FLUXES: GENERALLY NEGLECTED AT HIGH RE NUMBERS IN THE CONTEXT OF RANS.

iv) REYNOLDS STRESSES: GENERALLY MODELLED BY USING THE TURBULENT VISCOSITY:

$$\bar{\rho}\widetilde{\underline{u}''\underline{u}''} = -\mu_t\left(\nabla\tilde{\underline{u}} + \nabla\tilde{\underline{u}}^T - \frac{2}{3}\nabla\cdot\tilde{\underline{u}}\right) + \frac{2}{3}\bar{\rho}k \,, \quad \text{WITH } k = \frac{1}{2}\widetilde{|\underline{u}''^2|} \text{ THE TURBULENT KINETIC ENERGY.}$$

THE REASONING BEHIND $\mu_t$ HAS CLASSICALLY FOLLOWED ARGUMENTS THAT PARALLEL THOSE USED IN THE KINETIC THEORY OF GASES TO OBTAIN THE MOLECULAR VISCOSITY COEFFICIENT $\nu \sim a\lambda_a$, WITH $a$ THE SPEED OF SOUND AND $\lambda_a$ THE MEAN-FREE PATH (SEE FOR INSTANCE, PAGES 34-38 OF TENNEKES AND LUMLEY). IN ANALOGY TO THOSE, A MIXING-LENGTH MODEL IS TYPICALLY ENVISIONED IN A SHEAR LAYER IN WHICH TURBULENT TRANSPORT DISPLACES FLUID TRANSVERSALLY BY EDDY MOTION:



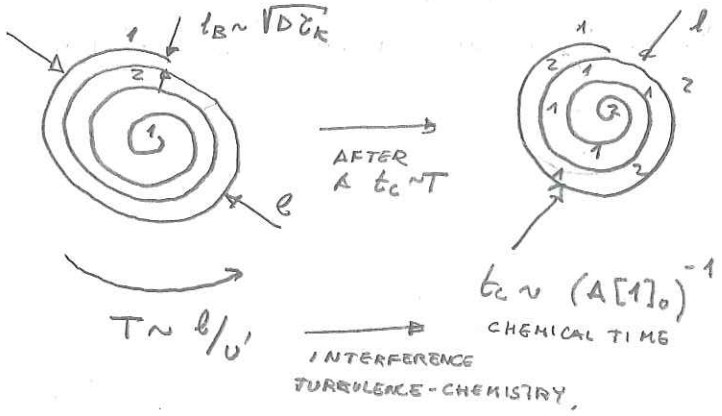

FOR SMALL DISPLACEMENTS IN $y$ (i.e. MUCH SMALLER THAN $U\left(\frac{dU}{dy}\right)^{-1}$), THEN $\tau_{xy} \sim \rho\overline{v'v'}\frac{\partial\bar{U}}{\partial y}$, AND DEFINING $\ell$ AS THE MIXING LENGTH BEYOND WHICH $\overline{v'v'}$ DECREASES TO ZERO (THE CORRELATION BETWEEN THE DISTANCE TRAVELLED AND THE VELOCITY DECREASES TO ZERO), THEN $\overline{v'v'} \sim \left(\overline{v'^2}\right)^{1/2}$ AND $\tau_{xy} \sim \rho\ell\left(\overline{v'^2}\right)^{1/2}\frac{\partial\bar{U}}{\partial y} = \rho\nu_t\frac{\partial\bar{U}}{\partial y}$, WITH $\nu_T \propto c_1\ell\left(\overline{v'^2}\right)^{1/2}$ THE EDDY VISCOSITY AND $c_1$ A CALIBRATED CONSTANT.

THIS APPROACH, HOWEVER, FAILS BECAUSE THE LARGEST EDDIES TEND TO HAVE SIZES COMPARABLE TO THE WIDTH OF THE FLOW, AND $\ell \sim U\left(\frac{dU}{dy}\right)^{-1}$, AND THE TRUNCATION OF THE TAYLOR EXPANSION INVOLVED IN THE DERIVATION ABOVE IS NOT JUSTIFIED.

IN GENERAL, HOWEVER, THE ASSERTION $\nu_t \sim$ CONSTANT $\cdot\, U'\ell$ IS USED OR IMPLICITLY ASSUMED, WHERE $U'$ AND $\ell$ ARE INTEGRAL QUANTITIES THAT ARE HARD TO IDENTIFY IN FLOWS WITH MULTIPLE INTEGRAL SCALES. $\Rightarrow$ $\frac{U'\ell}{\nu_t} \sim O(1)$ AND $\frac{\ell^2}{\nu_t} \sim \frac{\ell}{U'}$ $\Rightarrow$ INCREASED DIFFUSIVITY BY STIRRING!

THE GRADIENT HYPOTHESIS ALSO FAILS IN GENERAL TERMS IN THE PRESENCE OF SLOW CHEMISTRY SUCH AS THAT ENCOUNTERED IN IGNITION, EXTINCTION OR SLOW GENERATION OF COMPOUNDS ($NO_x$).

AS SOON AS THE LOCAL CHEMICAL TIMESCALE STARTS INTERACTING WITH TURNOVER TIMES IN THE INERTIAL RANGE, SCALAR FLUCTUATIONS ARE INDUCED IN THE ENERGY-CONTAINING EDDIES BY THE CHEMICAL REACTIONS. AS A RESULT, CHEMICAL-COMPOSITION VARIATIONS OCCUR IN INTEGRAL TIME SCALES OF THE VELOCITY FLUCTUATIONS, THE INTEGRAL TIME SCALE OF THE SCALAR FLUCTUATIONS BECOMES DEPENDENT ON CHEMISTRY, AND THE RATE OF TURBULENT TRANSPORT DEPENDS ON CHEMISTRY BY, FOR INSTANCE, A MODIFIED CHEMISTRY-DEPENDENT MASS DIFFUSIVITY (SEE CORRSIN 1961 AND PETER'S BOOK FOR DISCUSSION)




A POPULAR MODEL FOR OBTAINING THE TURBULENT VISCOSITY IS THE $k-\varepsilon$ MODEL, IN WHICH

$$\mu_t = \bar{\rho} C_\mu \tilde{k}^2/\tilde{\varepsilon} \quad \text{, OR EQUIVALENTLY,} \quad \nu_t = O\left(C_\mu u' l\right), \text{ WITH } C_\mu \sim 0.09 \text{ BY CALIBRATION}$$

WITH $\tilde{\varepsilon}$ AND $\tilde{k}$ OBTAINED BY THE $k-\varepsilon$ EQUATIONS: (PRODUCTION, DISSIPATION, MODELLED)

$$\bar{\rho}\frac{\partial \tilde{k}}{\partial t} + \bar{\rho}\tilde{u}\cdot\nabla\tilde{k} = \nabla\cdot\left(\frac{\bar{\rho}\nu_t}{\sigma_k}\nabla\tilde{k}\right) - \bar{\rho}\widetilde{u''u''}:\nabla\tilde{u} - \bar{\rho}\tilde{\varepsilon}$$

$$\bar{\rho}\frac{\partial \tilde{\varepsilon}}{\partial t} + \bar{\rho}\tilde{u}\cdot\nabla\tilde{\varepsilon} = \nabla\cdot\left(\frac{\bar{\rho}\nu_t}{\sigma_\varepsilon}\nabla\tilde{\varepsilon}\right) - C_{\varepsilon_1}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{u''u''}:\nabla\tilde{u} - C_{\varepsilon_2}\bar{\rho}\tilde{\varepsilon}^2/\tilde{k}$$

$C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k, \sigma_\varepsilon$ OBTAINED BY CALIBRATION.

WITH $\varepsilon = \nu\,\overline{\nabla u'':\nabla u''}$ THE DISSIPATION. (NOTE THAT FOR $\nu \to 0$ ($Re \to \infty$) THE DISSIPATION IS FINITE AND NON-ZERO). → SINGULAR LIMIT!

THIS MODEL IS GOOD FAR FROM WALLS (WHERE $T \to 0$ AS IS).

v) <u>MEAN SOURCE TERM</u> $\overline{\dot{w}_i}$ ⇒ CENTRAL TO TURBULENT COMBUSTION, CONSIDERED TO BE THE MAIN PROBLEM OF MOMENT METHODS IN TURBULENT COMBUSTION. FOR ILLUSTRATION PURPOSES, TAKE $\dot{w}_1 = A\rho Y_1 Y_2 e^{-T_a/T}$, WITH $\dot{w}_1 = \bar{\dot{w}}_1 + \dot{w}_1'$. THEN,

$$\dot{w}_1 = A(\bar{\rho}+\rho')(\tilde{Y}_1 + Y_1'')(\tilde{Y}_2 + Y_2'')\, e^{-\frac{T_a}{\tilde{T}+T''}},$$

WHICH EXEMPLIFIES THAT $\bar{\dot{w}}_1 \neq A\bar{\rho}\tilde{Y}_1\tilde{Y}_2 e^{-\frac{T_a}{\tilde{T}}}$ ⇒ THE MEAN OF THE FUNCTION IS NOT THE FUNCTION OF THE MEAN,

BUT $\bar{\dot{w}}_1 = A\bar{\rho}\tilde{Y}_1\tilde{Y}_2 e^{-\frac{T_a}{\tilde{T}}}\left[1 + \frac{\widetilde{Y_1''Y_2''}}{\tilde{Y}_1\tilde{Y}_2} + \frac{T_a}{\tilde{T}}\left(\frac{\widetilde{Y_1''T''}}{\tilde{Y}_1\tilde{T}} + \frac{\widetilde{Y_2''T}}{\tilde{Y}_2\tilde{T}}\right) + \dots\right]$ WHEN TAYLOR SERIES ARE USED.

THIS EQUATION LEADS TO SEVERAL DIFFICULTIES:

i) THE CORRELATIONS $\widetilde{Y_1''Y_2''}$, $\widetilde{Y_1''T''}$, $\widetilde{Y_2''T}$ NEED TO BE CLOSED.

ii) LARGE TRUNCATION ERRORS ARISE FROM THE TAYLOR EXPANSION BECAUSE OF THE EXPONENTIAL NON-LINEARITY UNLESS A LARGE NUMBER OF TERMS ARE RETAINED.

- <u>SCALAR DISSIPATION AND MIXING</u>.

CONSIDER (1) $\rho\frac{\partial Y_i}{\partial t} + \rho\underline{v}\cdot\nabla Y_i = \nabla\cdot(\rho D_i \nabla Y_i) + \dot{w}_i$ AND

(2) $\bar{\rho}\frac{\partial \tilde{Y}_i}{\partial t} + \bar{\rho}\tilde{\underline{v}}\cdot\nabla\tilde{Y}_i = \nabla\cdot\overline{(\rho D\nabla Y_i)} - \nabla\cdot\left(\bar{\rho}\widetilde{\underline{v}''\psi''}\right) + \bar{\rho}\tilde{S}_i$, WITH $\bar{\dot{w}}_i = \overline{\rho S_i} = \bar{\rho}\tilde{S}_i$

SINCE $\widetilde{Y_i''^2} = \widetilde{(Y_i - \tilde{Y}_i)^2} = \tilde{Y}_i^2 - \tilde{Y}_i^2$, MULTPLYING (1) BY $2Y_i$:

$$\frac{\partial}{\partial t}(\rho Y_i^2) + \nabla\cdot(\rho\underline{v}Y_i^2) = 2Y_i\nabla\cdot(\rho D_i\nabla Y_i) + 2Y_i\rho\dot{S}_i \quad \text{AND AVERAGING:}$$

$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{Y_i''^2}\right) + \nabla\cdot\left(\bar{\rho}\tilde{u}\widetilde{Y_i''^2}\right) = 2\overline{Y_i\nabla\cdot(\rho D_i\nabla Y_i)} + 2\bar{\rho}\widetilde{\dot{\omega}S}$ IS OBTAINED. NOTICE THAT $\nabla\cdot(\bar{\rho}\tilde{u}\widetilde{Y_i''^2}) = \nabla\cdot\left[\bar{\rho}(\tilde{u}+u'')(\widetilde{Y_i}+Y_i'')^2\right] = \nabla\cdot(\bar{\rho}\tilde{u}\widetilde{Y_i''^2}) + \nabla\cdot(\bar{\rho}\tilde{u}\widetilde{Y_i''^2}) + 2\nabla\cdot\left[\tilde{u}\widetilde{Y_i}\bar{\rho}\widetilde{Y_i''}\right] +$ $+ \nabla\cdot\left(\bar{\rho}\widetilde{u''Y_i''^2}\right) + \nabla\cdot(\bar{\rho}\widetilde{u''Y_i''^2}) + 2\nabla\cdot\left(\bar{\rho}\widetilde{Y_i}\widetilde{u''Y_i''}\right)$.

THEN, $\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{Y_i''^2}\right) + \nabla\cdot(\bar{\rho}\tilde{u}\widetilde{Y_i''^2}) + \bar{\rho}\widetilde{u''}\cdot\nabla\widetilde{Y_i''^2} + \nabla\cdot\left(\bar{\rho}\widetilde{u''Y_i''^2}\right) + 2\nabla\cdot\left(\bar{\rho}\widetilde{Y_i}\widetilde{u''Y_i''}\right) =$

$= 2Y_i\nabla\cdot(\rho D_i\nabla Y_i) + 2\bar{\rho}\widetilde{Y_i\dot{S}_i}$. (4)

ALSO MULTIPLYING (2) BY $2\widetilde{Y_i}$:

$\frac{\partial}{\partial t}\left(\bar{\rho}\widetilde{Y_i}^2\right) + \nabla\cdot\left(\bar{\rho}\tilde{u}\widetilde{Y_i}^2\right) = 2\widetilde{Y_i}\nabla\cdot\left(\overline{\rho D_i\nabla Y_i}\right) - 2\widetilde{Y_i}\nabla\cdot\left(\bar{\rho}\widetilde{u''Y_i''}\right) + 2\widetilde{Y_i}\bar{\rho}\widetilde{\dot{S}}$ (5).

SINCE, IN EQ. (5), $2\widetilde{Y_i}\nabla\cdot\left(\bar{\rho}\widetilde{u''Y_i''}\right) = 2\nabla\cdot\left(\bar{\rho}\widetilde{Y_i}\widetilde{u''Y_i''}\right) - 2\bar{\rho}\widetilde{u''Y_i''}\nabla\widetilde{Y_i}$, AND

$2\overline{Y_i\nabla\cdot(\rho D_i\nabla Y_i)} - 2\widetilde{Y_i}\nabla\cdot\left(\overline{\rho D_i\nabla Y_i}\right) = 2\overline{\left(\widetilde{Y_i}+Y_i''\right)\nabla\cdot\left(\rho D_i\nabla\left(\widetilde{Y_i}+Y_i''\right)\right)} - 2\widetilde{Y_i}\nabla\cdot\left(\overline{\rho D_i\nabla(\widetilde{Y_i}+Y_i'')}\right)$

$= 2\widetilde{Y_i}\nabla\cdot\left(\overline{\rho D_i\nabla\left(\widetilde{Y_i}+Y_i''\right)}\right) - 2\widetilde{Y_i}\nabla\cdot\left(\overline{\rho D\nabla\left(\widetilde{Y_i}+Y_i''\right)}\right) + 2\overline{Y_i''\nabla\cdot\left(\rho D_i\nabla\left(\widetilde{Y_i}+Y_i''\right)\right)} =$

$= 2\overline{Y_i''\nabla\cdot\left(\rho D_i\nabla\widetilde{Y_i}\right)} + 2\overline{Y_i''\nabla\cdot\left(\rho D_i\nabla Y_i''\right)} = 2\overline{Y_i''\nabla\cdot\left(\rho D_i\nabla\widetilde{Y_i}\right)} + 2\nabla\cdot\left(\overline{\rho D_i Y_i''\nabla Y_i''}\right)$

$- 2\overline{\rho D_i\left(\nabla Y_i''\right)^2} = \nabla\cdot\left(\overline{\rho D_i\nabla Y_i''^2}\right) - 2\overline{\rho D_i\left(\nabla Y_i''\right)^2} + 2\overline{Y_i''\nabla\cdot\left(\rho D_i\nabla\widetilde{Y_i}\right)}$.

AND $2\bar{\rho}\widetilde{Y_i\dot{S}} - 2\bar{\rho}\widetilde{Y_i}\widetilde{\dot{S}_i} = 2\bar{\rho}\widetilde{Y_i''\dot{S}_i''}$, THEN SUBSTRACTING (5) FROM (4) AND USING THE IDENTITIES ABOVE, THE SCALAR-VARIANCE EQUATION ②

$$\bar{\rho}\frac{\partial\widetilde{Y_i''^2}}{\partial t} + \bar{\rho}\tilde{u}\cdot\nabla\widetilde{Y_i''^2} = -\nabla\cdot\left(\bar{\rho}\widetilde{u''Y_i''^2}\right) - 2\bar{\rho}\widetilde{u''Y_i''}\nabla\widetilde{Y_i} + 2\overline{Y_i''\nabla\cdot\left(\rho D_i\nabla\widetilde{Y_i}\right)} +$$
$$+ \nabla\cdot\left(\overline{\rho D_i\nabla Y_i''^2}\right) - 2\overline{\rho D_i\left(\nabla Y_i''\right)^2} + 2\bar{\rho}\widetilde{Y_i''\dot{S}_i''}$$

IS OBTAINED

WITH ① = TURBULENT TRANSPORT, ② = PRODUCTION, ③ MOLECULAR DIFFUSION → NOTICE THAT $\nabla\widetilde{Y_i} \neq 0$ IMPLIES THAT $\widetilde{Y_i''^2} \neq 0$ IN TURBULENT FLOWS!

④ SCALAR DISSIPATION, ⑤ CHEMICAL REACTION. THE TERMS ①, ②, ④ AND ⑤ ARE UNCLOSED.

THE SCALAR DISSIPATION ALWAYS ACTS AS A SINK AND DETERMINES HOW QUICKLY THE SCALAR FLUCTUATIONS DECAY. ABSENCE OF FLUCTUATIONS IMPLIES A WELL-MIXED FLUID AND HENCE WE CAN UNDERSTAND THE SCALAR DISSIPATION AS A MEASURE OF THE RATE AT WHICH MIXING OCCURS.

$$\rightarrow \bar{\rho}\widetilde{\chi} = \overline{\rho D\left(\nabla Y_i\right)^2} = \overline{\rho D\left[\nabla\left(\widetilde{Y_i}+Y''\right)\right]^2} = \bar{\rho}D\left(\nabla\widetilde{Y_i}\right)^2 + 2\overline{\rho D\nabla Y_i''}\nabla\widetilde{Y_i} +$$
$$+ \overline{\rho D\nabla Y_i''\nabla Y_i''} \approx \overline{\rho D\left(\nabla Y_i''\right)^2} \quad \text{SCALAR DISSIPATION}$$

↳ AT HIGH REYNOLDS NUMBERS THE GRADIENTS OF THE SCALARS ARE MUCH STEEPER AT THE SMALL SCALES THAN AT THE LARGE SCALES

HIGH RATES OF MOLECULAR MIXING (HIGH $\chi$) IMPLY HIGH RATES OF CHEMICAL REACTIONS (IF THE TEMPERATURE IS HIGH ENOUGH). THE SCALAR DISSIPATION RATE DIRECTLY MEASURES THE DECAYING SPEED OF FLUCTUATIONS VIA TURBULENT MICROMIXING. MODELLING $\chi$ IS AN EXTREMELY IMPORTANT TOPIC IN COMBUSTION. A USUAL MODEL IS

$$\chi \propto C_\chi\frac{\widetilde{Y_i''^2}}{\tau} \quad \text{WITH } \tau = k/\varepsilon \text{ AND } C_\chi \sim 2 \text{ A CONSTANT}$$

THE IDEA BEHIND THIS EXPRESSION IS THAT "ENERGY" OF MAGNITUDE $\widetilde{Y_i''^2}$ MUST BE TRANSFERRED TO THE SMALL SCALES AT A RATE DICTATED BY THE LARGE-EDDY TIMESCALE $\tau$. NOTICE THAT $\varepsilon$, AS WELL AS $\chi$ ARE INDEPENDENT OF $D$. THIS MODEL STATES THAT THE SCALAR AND VELOCITY-FLUCTUATION TIME SCALES ARE SIMILAR. → NOT GOOD IN COMPLEX BURNERS.

## - SCALAR DISSIPATION RATE IN PLANAR MIXING LAYERS



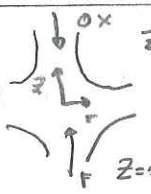

$$\frac{\partial \xi}{\partial t} = D\frac{\partial^2 \xi}{\partial y}$$

WITH $\xi = 0,\ y>0\ \ t=0$ AND $\xi = 1,\ y<0,\ t=0$ ; AND $\xi \to 1$ AT $y \to -\infty\ \ t>0$, $\xi \to 0$ AT $y \to +\infty\ \ t>0$

THEN $\xi = \frac{1}{2}\,\mathrm{erfc}(\eta)$ WITH $\eta = y/\sqrt{4Dt}$ AND $\chi|_{y=0} = D\left(\frac{d\xi}{dy}\right)^2_0 = \frac{1}{4\pi t}$

WITH $\chi \neq f(D)$ AND $\chi \to 0$ AS $t \to \infty$

## - STEADY COUNTERFLOW MIXING LAYER




$$D\frac{d^2 Z}{dz^2} = -A z \frac{dZ}{dz}$$ WITH $A$ = STRAIN RATE

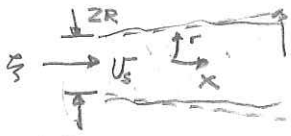
$z \to \infty \quad Z = 0$

$z \to -\infty \quad Z = 1$

THEN $Z = \frac{1}{2}\,\mathrm{erfc}\left(\frac{\eta}{\sqrt{2}}\right)$ WITH $\eta = \frac{z}{\sqrt{D/A}}$

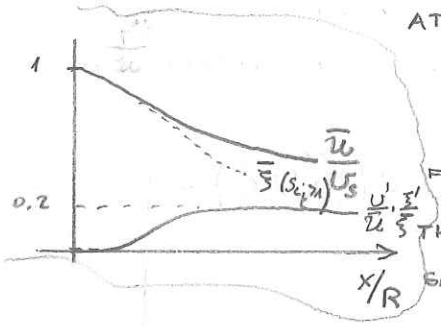
AND $\chi = D\left(\frac{dZ}{dz}\right)^2 = \frac{A}{2\pi}$ AT $\eta = 0$ (MAX SCALAR DISSIPATION)

## - MIXING IN TURBULENT JETS




CONTINUITY: $\frac{\partial \bar{U}}{\partial x} + \frac{1}{r}\frac{\partial}{\partial r}(r\bar{v}) = 0$

X-MOMENTUM: $\bar{U}\frac{\partial \bar{U}}{\partial x} + \bar{v}\frac{\partial \bar{U}}{\partial r} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\overline{u'v'}\right) = \frac{\nu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \bar{U}}{\partial r}\right)$



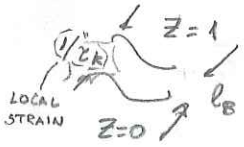

AT $Re = \frac{U_s R}{\nu} \gg 1$, THE INTEGRATION OF THE MOMENTUM EQUATION YIELDS

$$\frac{d}{dx}\int_0^\infty r\bar{U}^2 dr = -\left[r\bar{U}\bar{v} + r\overline{u'v'}\right]_0^\infty = 0$$ , SO THAT THE MOMENTUM FLUX $M = \int_0^\infty 2\pi r \bar{U}^2 dr$ = CONSTANT $\rightarrow \bar{U} r^2 \sim \tilde{u} r_{1/2}^2 \sim$ CONST, WITH $\tilde{u}$ THE MEAN BULK VELOCITY AND $r_{1/2}$ THE JET OPENING. SELF-SIMILAR ANALYSES SHOW THAT $\frac{dr_{1/2}}{dx}$ = CONST (SEE POPE), WITH $r_{1/2} \sim x$ AND $\tilde{u} \sim 1/x$

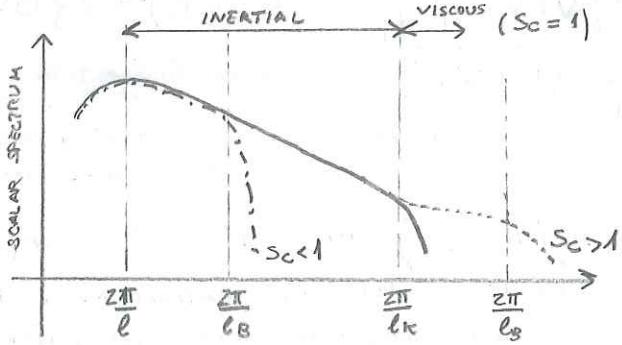
⇒ EDDY-DIFFUSIVITY: $\mathcal{D}_T \sim r^{1/2}\tilde{u} \sim$ CONST $\sim R U_s$, THUS, INCREASING $U_s$ INCREASES $\mathcal{D}_T$ AND THEREFORE INCREASES THE MIXING RATE ⇒ THE LENGTH OF A TURBULENT FLAME IS INDEPENDENT OF THE NOZZLE VELOCITY.

## - LENGTH SCALES AND SPECTRA IN MIXING

IN TURBULENT FLOWS, THE LENGTH SCALE BEYOND WHICH MOLECULAR MIXING STARTS TO HAPPEN IS THE BATCHELOR SCALE $\ell_B$, WHICH IS A DIFFUSION THICKNESS ACCROSS A KOLMOGOROV TIME:




$$\ell_B \simeq (D\tau_k)^{1/2} = \ell_k S_c^{-1/2}$$ , WITH $S_c = \frac{\nu}{D}$ THE MOLECULAR SCHMIDT NUMBER.




FOR $S_c = 1 \rightarrow \ell_B = \ell_k$

$S_c < 1 \rightarrow \ell_B > \ell_k$ ($H_2$-AIR COMBUSTION)

$S_c > 1 \rightarrow \ell_B < \ell_k$ (LIQUIDS)

NOTE THAT AS $D \to 0$, THE BATCHELOR LENGTH GOES TO ZERO, BUT THE MICROSCALE DIFFUSION TIME $\tau_B \sim \ell_B^2/D$ GOES TO INFINITY. IN PARTICULAR, FOR $S_c \sim Re_\ell^{2/3}$ ONE OBTAINS THAT $\tau_B \sim T$

⇒ EXTRAPOLATION OF GASEOUS COMBUSTION RESULTS TO LIQUID-COMBUSTION CASES HAS TO BE MADE WITH GREAT CARE.

⇒ MOLECULAR MIXING OCCURS WHERE $\chi$ IS HIGH, IN LAYERS OF THICKNESS OF $O(\ell_B)$ → SEE FIG 15, AND THESE ZONES ARE LIKELY WHERE REACTION LIES.

⇒ STIRRING VS MIXING:

"STIRRING": MECHANICAL PROCESS WHEREBY FLUIDS ARE DISTRIBUTED MORE UNIFORMLY WITHIN A GIVEN DOMAIN → PROCESS OF STRETCHING OF INTERMATERIAL AREA.

"MIXING": PROCESS OF DIFFUSION OF SUBSTANCES ACROSS INTERMATERIAL AREAS.

⇒ MIXING DEPENDS ON MATERIAL PROPERTIES, WHEREAS STIRRING IS A PURELY KINEMATICAL ASPECT THAT DEPENDS ON FLOW PARAMETERS. IN FACT, IT IS POSSIBLE TO STIR FLUIDS THAT DO NOT MIX AT ALL!

## SEPARATION OF SCALES IN TURBULENT COMBUSTION (SEE FIG 14)

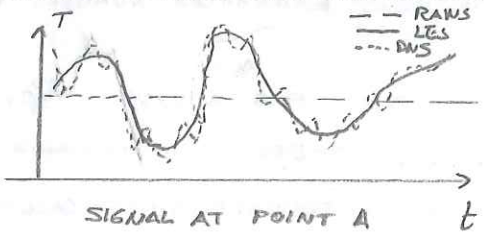
COMBUSTION REQUIRES THAT FUEL AND OXIDIZER MUST BE MIXED AT THE MOLECULAR LEVEL FOR CHEMICAL REACTIONS TO OCCUR. HOW THIS TAKES PLACE IN TURBULENT COMBUSTION DEPENDS ON THE TURBULENT MIXING PROCESS. THE GENERAL VIEW IS THAT ONCE A RANGE OF DIFFERENT SIZE EDDIES COME TOGETHER, STRAIN AND SHEAR AT THE INTERFACE BETWEEN THE EDDIES ENHANCE MIXING. DURING THE EDDY BREAK UP, THE SHEAR AND STRAIN INCREASE, THEREBY STEEPENING THE CONCENTRATION GRADIENTS AT THE INTERFACE BETWEEN REACTANTS, WHICH IN TURN ENHANCES THEIR MOLECULAR INTERDIFFUSION. MOLECULAR MIXING THEREFORE TAKES PLACE AT THE INTERFACE BETWEEN SMALL EDDIES. THIS PROCESS IS MODIFIED BY CHEMICAL REACTIONS, SINCE THEY STEEPEN THE GRADIENTS EVEN MORE.

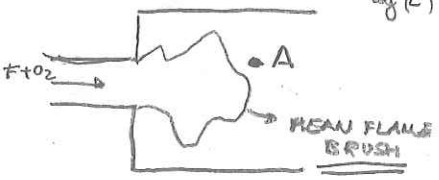
IF THE CHEMICAL SCALES WOULD INTERACT WITH THE INERTIAL RANGE, NO SIMPLE SCALING LAWS AS IN CLASSICAL TURBULENCE THEORY (I.E. KOLMOGOROV UNIVERSAL EQ.-THEORY) WOULD BE POSSIBLE AND THERE WOULD NOT BE ASYMPTOTIC INVARIANCE (I.E. INDEPENDENCE OF $\mathcal{D}$ AT $Re_t \to \infty$)

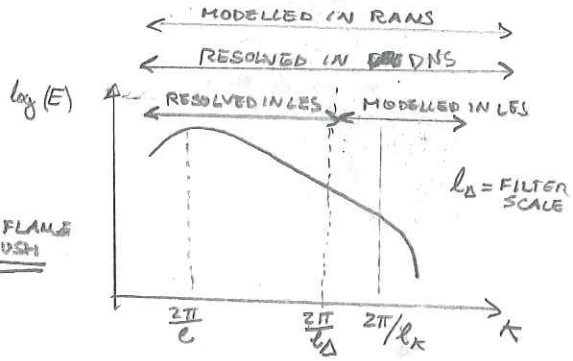
THE SCALE-SEPARATION HYPOTHESIS IS BASED ON CHEMISTRY-INDEPENDENT INERTIAL RANGE. ($t_c \to 0$)

IGNITION AND EXTINCTION ARE EXCEPTION TO THIS SITUATION SINCE THE ASSOCIATED TIME SCALES ARE SLOW

### COMPUTATIONAL APPROACHES FOR TURBULENT COMBUSTION




COMPUTATIONAL COST ↓

RANS: FIRST APPROACH DEVELOPED. THE REYNOLDS- OR FAVRE-AVERAGE EQUATIONS REQUIRE CLOSURE RULES (TURBULENCE MODEL FOR THE FLOW + TURBULENT-COMBUSTION MODEL). THE SOLUTIONS PROVIDE TIME-AVERAGED OR ENSEMBLE-AVERAGED QUANTITIES. ⇒ RESOLUTION: $\Delta x \sim 1\text{-}5$ mm.

LES: THE LARGE SCALES ARE CALCULATED WHEREAS THE SMALLEST ONES ARE MODELLED USING SUBGRID SCALE MODELS. THE LES EQUATIONS ARE OBTAINED BY FILTERING THE INSTANTANEOUS N-S EQUATIONS. NOTE HOWEVER, THAT IF USE OF NON-UNIFORM GRIDS IS MADE, THE LES EQUATIONS ARE NOT EXACT EVEN PRIOR TO MODELLING BECAUSE OF PERMUTATION ERRORS BETWEEN THE FILTERING OPERATOR AND THE SPATIAL GRADIENTS. LES CAPTURES LOW-FREQUENCY (ENERGY-CONTAINING) VARIATIONS OF THE MAGNITUDES → MUCH BETTER THAN RANS FOR THE STUDY OF COMBUSTION INSTABILITIES. ⇒ COST IS 100 TO 1000 TIMES HIGHER THAN RANS.

DNS: FULL NS ARE SOLVED WITHOUT MODELLING AT SMALL SCALES. DNS PROVIDES ALL TIME VARIATIONS. LIMITED TO RELATIVELY SIMPLE SCENARIOS. ⇒ RESOLUTION: $\Delta x \sim 10\text{-}50\ \mu$m

⇒ AVERAGED FIELDS FOR COMPARISONS WITH RANS CAN BE OBTAINED EXPERIMENTALLY BY USING SINGLE-POINT MEASUREMENTS (LDV, THERMOCOUPLE, SINGLE POINT RAMAN SCATTERING,...).

## DIRECT NUMERICAL SIMULATIONS IN TURBULENT COMBUSTION

- ONLY FEASIBLE IN SIMPLE CASES. OFTEN USED IN ANALYSES EXCLUDING THERMAL EXPANSION OR ASSUMING LOW MACH NUMBERS.

- RESOLUTION REQUIREMENTS: DIRECT-NUMERICAL SIMULATIONS GRIDS MUST BE SUCH THAT i) THE CALCULATION IS PERFORMED IN THE LARGEST POSSIBLE DOMAIN (I.E. LARGER THAN THE INTEGRAL LENGTH SCALE) IN ORDER TO HAVE MEANINGFUL STATISTICS, ii) THE SMALLEST SCALES ARE RESOLVED.

IF $L^3$ IS THE MESH SIZE AND $N^3$ IS ITS NUMBER OF POINTS, THEN $\Delta x = \frac{L}{N}$ REPRESENTS THE STEP SIZE. THUS, CONDITION i) IS SATISFIED WHEN $L > \ell$. SINCE THE KOLMOGOROV LENGTH IS $\ell_K \sim \ell\, Re_\ell^{-3/4}$ AND $\Delta x$ MUST BE SMALLER THAN $\ell_K$, THEN ii) AND i) ARE SATISFIED SIMULTANEOUSLY WHEN

$$\left.\begin{aligned} \ell &< N\Delta x \\ \Delta x &< \ell_K \end{aligned}\right\} \Rightarrow \frac{\ell}{\ell_K} < N \quad \text{OR EQUIVALENTLY, WHEN} \quad \boxed{N > Re_\ell^{3/4}}$$

IF, HOWEVER, THE FLAME THICKNESS $\delta_L^0$ (FOR PREMIXED COMBUSTION) IS SMALLER THAN THE KOLMOGOROV THICKNESS (AS PER USUAL), THEN THE ADDITIONAL REQUIREMENT ii) $\Delta x < \delta_L^0$ NEEDS TO BE MET. IN PARTICULAR, IF $N_f$ IS THE NUMBER OF POINTS ACCROSS THE FLAME ($N_f$ NEEDS TO BE OF ORDER 100 FOR PROPER RESOLUTION OF THE REACTIVE-DIFFUSIVE ZONE), THEN $\delta_L^0 \sim N_f \Delta x$ AND $\boxed{\frac{\ell}{\delta_L^0} < \frac{N}{N_f}}$ FOR SATISFYING CONDITIONS i) AND ii) (WHICH AUTOMATICALLY SATISFY CONDITION ii) IF $\delta_L^0 < \ell_K$. SINCE $\frac{\ell}{\delta_L^0} \sim \frac{\ell}{\delta_L^0}\cdot\frac{u'}{u'}\cdot\frac{\nu}{\nu}\cdot\frac{s_L^0}{s_L^0}\cdot\frac{\delta_L^0}{u'} = Re_\ell\left(\frac{s_L^0}{u'}\right)$ AND $\frac{\ell}{\delta_L^0} \sim \frac{u'T}{s_L^0(t_c)} = \frac{u'}{s_L^0}\cdot Da$, WITH $Da = \frac{T}{t_c}$ THE TURBULENT DAMKÖHLER NUMBER, THEN

$$\left(\frac{\ell}{\delta_L^0}\right)^2 = Re_\ell Da < \left(\frac{N}{N_f}\right)^2 \Rightarrow$$

NOTE THAT FOR A GIVEN $N_f$, $N$ AND $Da$, THERE IS A MAXIMUM $Re_\ell$ THAT CAN BE SIMULATED NUMERICALLY.

CHEMICAL TIMES, SEE REVERSE PAG. 7

THE TIME STEP IN DIRECT NUMERICAL SIMULATIONS IS TYPICALLY LIMITED BY THE CHEMICAL TIMESTEP.

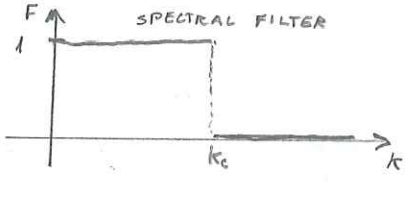
## LARGE-EDDY SIMULATIONS

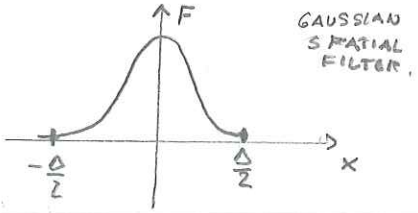
IN LES THE VARIABLES ARE NOT AVERAGED BUT FILTERED IN THE WAVE-NUMBER SPACE OR IN THE PHYSICAL SPACE. THE FILTERED VERSION OF THE QUANTITY $\phi$ IS DEFINED AS

$$\bar{f}(\underline{x}) = \int f(\underline{x}')F(\underline{x}-\underline{x}')\,dx' \qquad (\rho = \text{CONST})$$

$$\text{OR} \quad \bar{\rho}\tilde{\bar{f}}(\underline{x}) = \int \rho f(\underline{x}')F(\underline{x}-\underline{x}')\,dx' \qquad (\rho \neq \text{CONST}).$$

DIFFERENT FILTERS EXIST THAT SUPPRESS FREQUENCY COMPONENTS LARGER THAN A CUTOFF FREQUENCY OR SMOOTH VARIABLES BELOW A PARTICULAR SIZE.



THEN $\phi = \bar{\phi} + \phi'$, WITH $\bar{\phi}$ SOLVED IN THE NUMERICAL SIMULATION AND $\phi'$ THE SUBGRID-SCALE PART THAT IS MODELLED. THE FILTERED NS EQUATIONS ARE

$$\begin{cases} \dfrac{\partial \bar{\rho}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}) = 0 \\ \dfrac{\partial}{\partial t}(\bar{\rho}\tilde{\underline{u}}) + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{\underline{u}}) = -\nabla\bar{P} + \nabla\cdot\left[\bar{\underline{\tau}} - \bar{\rho}(\widetilde{\underline{u}\underline{u}} - \tilde{\underline{u}}\tilde{\underline{u}})\right] \\ \dfrac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_k) + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{Y}_k) = \nabla\cdot\left[\overline{\rho D_k \nabla Y_k} - \bar{\rho}(\widetilde{\underline{u}Y_k} - \tilde{\underline{u}}\tilde{Y}_k)\right] + \overline{\dot{w}_k} \\ \dfrac{\partial}{\partial t}(\bar{\rho}\tilde{h}_s) + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{h}_s) = \dfrac{\overline{Dp}}{Dt} + \nabla\cdot\left[\overline{\lambda\nabla T} - \bar{\rho}(\widetilde{\underline{u}h_s} - \tilde{\underline{u}}\tilde{h}_s)\right] + \overline{\underline{\tau}:\nabla\underline{u}} \\ \qquad - \nabla\cdot\left(\overline{\rho\sum_{k=1}^{N} \underline{V}_k Y_k h_{s,k}}\right) - \overline{\sum_{k=1}^{N} h_k^0 \dot{w}_k}, \quad \text{WITH} \quad \dfrac{\overline{Dp}}{Dt} = \dfrac{\partial\bar{p}}{\partial t} + \overline{\underline{u}\cdot\nabla p} \end{cases}$$

⇒ APPLY FILTERING OPERATOR $\bar{\rho}\tilde{\phi} = \int \rho\phi F(x-x')dx$

NOTICE THAT, IN ORDER TO OBTAIN THESE EQUATIONS, ONE NEEDS TO COMMUTE FILTER AND TIME DERIVATIVE OPERATORS, WHICH IS NOT A VALID PROCEDURE WHEN THE FILTER SIZE VARIES IN TIME AND SPACE. IN THESE EQUATIONS, THE UNRESOLVED TURBULENT FLUXES, THE FILTERED REACTION RATE, THE FILTERED MOLECULAR FLUXES AND THE PRESSURE VELOCITY TERM NEED TO BE MODELLED. IN LES, LARGE-SCALE TURBULENT MOTIONS ARE NUMERICALLY RESOLVED, AND THEREFORE SIMILARITY ASSUMPTIONS CAN BE USED TO ESTIMATE THE EFFECTS OF THE SMALL SCALES.

MODELLING OF UNRESOLVED FLUXES IN LES

- SMAGORINSKY MODEL: $T_{ij} - \frac{\delta_{ij}}{3}T_{kk} = -\nu_t\left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial\tilde{u}_k}{\partial x_k}\right) = -2\nu_t\left(\tilde{S}_{ij} - \frac{\delta_{ij}}{3}\tilde{S}_{kk}\right)$

OR EQUIVALENTLY: $\underline{\underline{\mathcal{T}}} - \frac{\delta_{ij}}{3}\overline{\overline{T}} = -2\nu_t\left(\tilde{\underline{\underline{S}}} - \frac{2}{3}\nabla\cdot\tilde{\underline{u}}\right)$, $\tilde{\underline{\underline{S}}} = \frac{1}{2}\left(\nabla\tilde{\underline{u}} + \nabla\tilde{\underline{u}}^T\right)$ THE FILTERED STRAIN TENSOR WITH

FOR COMPRESSIBLE FLOWS: $T_{kk} = 2C_I\bar{\rho}\Delta^2|\tilde{S}|^2$

WHERE $\nu_t$ IS A SUBGRID-SCALE VISCOSITY MODELLED AS

$$\nu_t = (C_s\Delta)^2\left(2\tilde{\underline{\underline{S}}}:\tilde{\underline{\underline{S}}}\right)^{1/2}$$

HERE $\underline{\underline{\mathcal{T}}} = \widetilde{\underline{u}\underline{u}} - \tilde{\underline{u}}\tilde{\underline{u}}$

WITH $C_s$ A SMAGORINSKY CONSTANT THAT DEPENDS ON THE FLOW CONFIGURATION. THE CONSTANT $C_s$ CAN BE OBTAINED DYNAMICALLY BY USING, FOR INSTANCE, THE GERMANO IDENTITY, WHICH HAS THE OBJECTIVE TO ESTIMATE SMALL SCALE DISSIPATION FROM THE KNOWLEDGE OF THE RESOLVED EDDIES. IN THE GERMANO DYNAMIC MODEL, A TEST FILTER OF SIZE $\hat{\Delta}$ LARGER THAN THE LES FILTER $\Delta$, IS INTRODUCED. THE UNRESOLVED SUBGRID MOMENTUM FLUXES ARE $\mathcal{T} = \widetilde{\underline{u}\underline{u}} - \tilde{\underline{u}}\tilde{\underline{u}}$, AND THE UNRESOLVED FLUXES AT THE TEST LEVEL ARE $\mathcal{T}^* = \widehat{\underline{u}\underline{u}} - \hat{\underline{u}}\hat{\underline{u}}$, THE TWO PREVIOUS RELATIONS CAN BE COMBINED TO GIVE THE GERMANO IDENTITY $= \mathcal{T}^* - \hat{\mathcal{T}} = \widehat{\tilde{u}\tilde{u}} - \hat{\tilde{u}}\hat{\tilde{u}} = \mathcal{L}$, WITH $\mathcal{L}$ DETERMINED BY FILTERING THE RESOLVED LES VELOCITY FIELD $\tilde{u}$ AT THE TEST LEVEL $\hat{\Delta}$. USING THE SMAGORINSKY MODEL FOR $\mathcal{T}^*$ AND $\mathcal{T}$ LEADS TO:

$$\mathcal{T} - \frac{\delta}{3}\mathcal{T} = -2(C_s\Delta)^2\left(2\tilde{\underline{\underline{S}}}:\tilde{\underline{\underline{S}}}\right)^{1/2}\left(\tilde{\underline{\underline{S}}} - \frac{2}{3}\nabla\cdot\tilde{\underline{u}}\right) = -2C_s^2\alpha$$

$$\mathcal{T}^* - \frac{\delta}{3}\mathcal{T}^* = -2(C_s\hat{\Delta})^2\left(2\hat{\tilde{\underline{\underline{S}}}}:\hat{\tilde{\underline{\underline{S}}}}\right)^{1/2}\left(\hat{\tilde{\underline{\underline{S}}}} - \frac{2}{3}\nabla\cdot\hat{\tilde{\underline{u}}}\right) = -2C_s^2\beta$$

THEN THE GERMANO IDENTITY BECOMES:

$$\mathcal{L} - \frac{\delta}{3}\mathcal{L} = 2C_s^2(\alpha - \beta), \quad \text{WITH } C_s(\underline{x},t) \text{ OBTAINED BY OPTIMIZATION PROCEDURES}$$

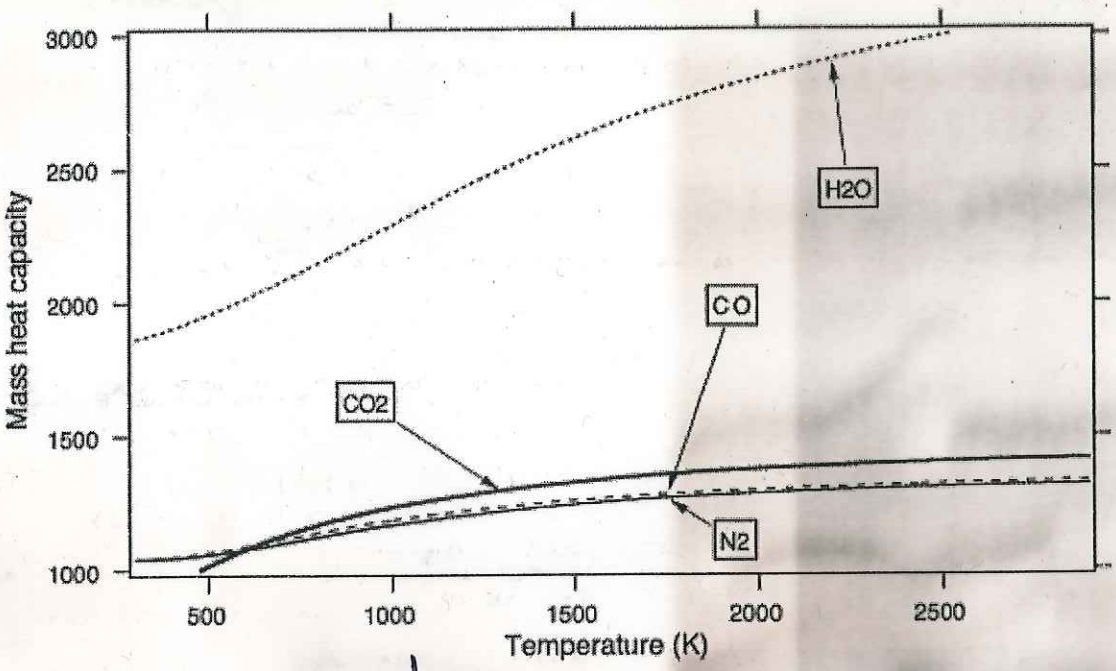
FROM THIS IDENTITY (GERMANO, PIOMELLI, MOIN + CABOT, 1991)

THE UNRESOLVED SCALAR TRANSPORT IS SIMILARLY WRITTEN: $\underline{\widetilde{u}\widetilde{Y}_i} - \underline{\widetilde{u}}\,\widetilde{Y}_i = -\frac{\nu_t}{Sc_t}\nabla\widetilde{Y}_i$

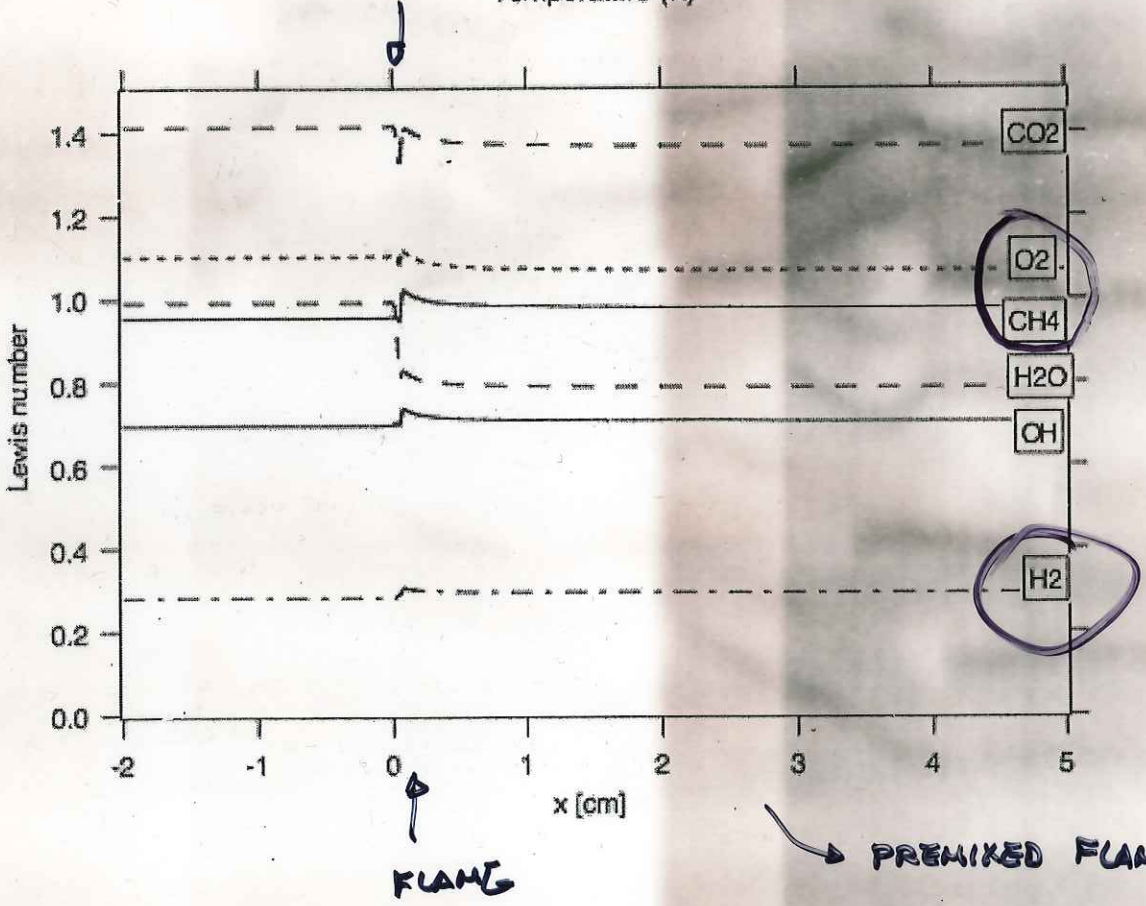
IN ANY CASE, THE NUMERICS SHOULD BE GOOD ENOUGH SUCH THAT THE SUBGRID MODELS ARE NOT OFFSET BY NUMERICAL DISSIPATION.

FIG 1

POINSOT + VEYNANTE (2005)




$C_p$ [J/kgK]



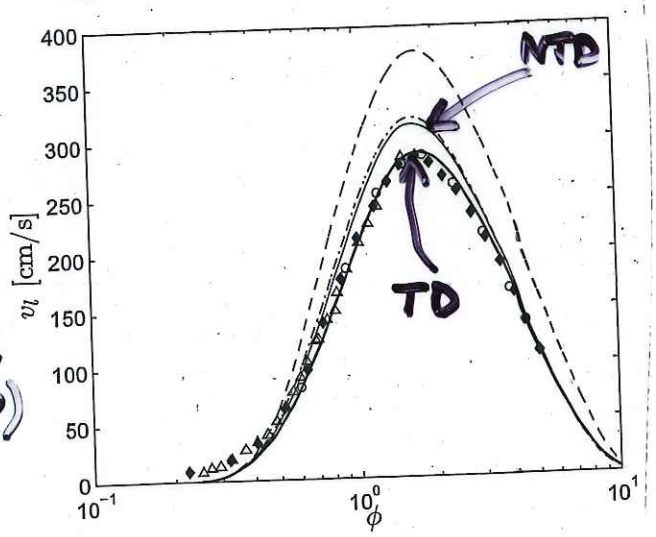

$Le_i = \frac{D_T}{D_i}$

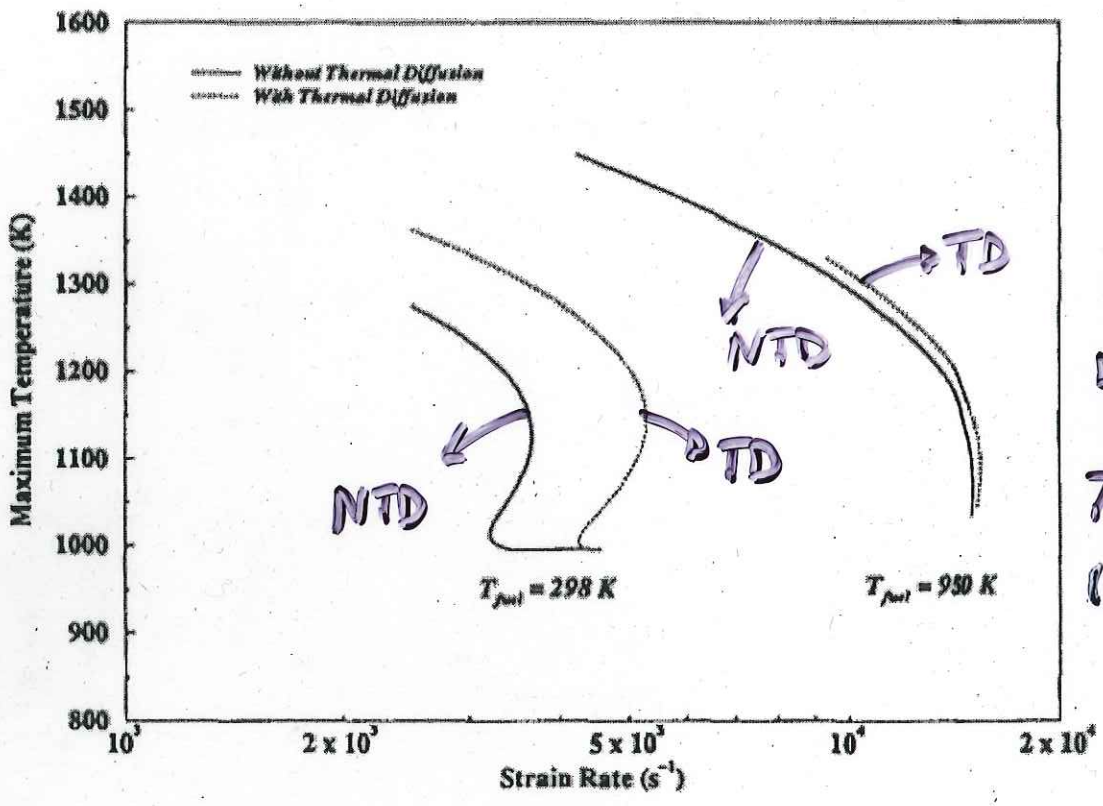
FLAME

→ PREMIXED FLAMES

FIG 2

FLAME SPEED
$H_2/O_2$ . 1 ATM
300 K
(GALISTEO, 2010)

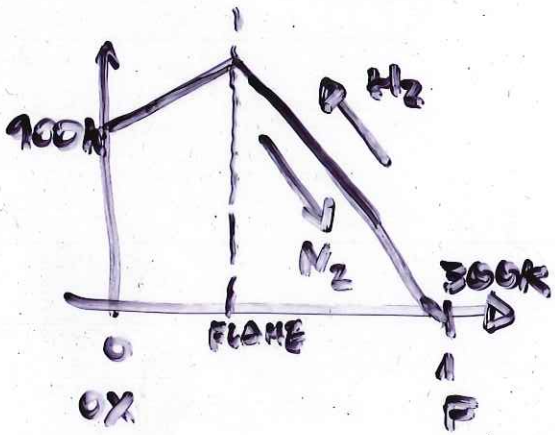



$H_2/O_2$
DIFFUSION
FLAME

$T_{ox} \sim 900$ K

(BALAKRISHNAN
ET AL. 1995)



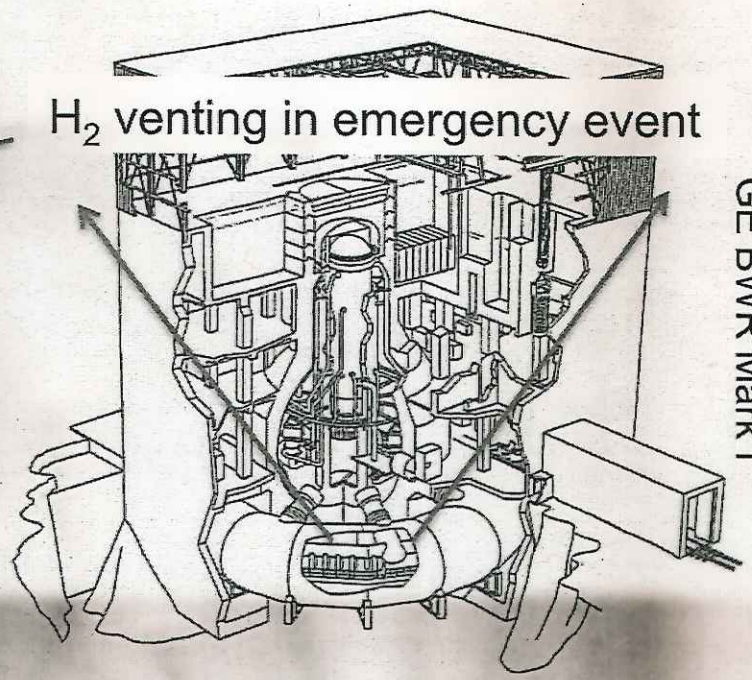

THERMAL DIFFUSION

# Motivations

Energy: Explosive bounds of $H_2$ in nuclear power plants



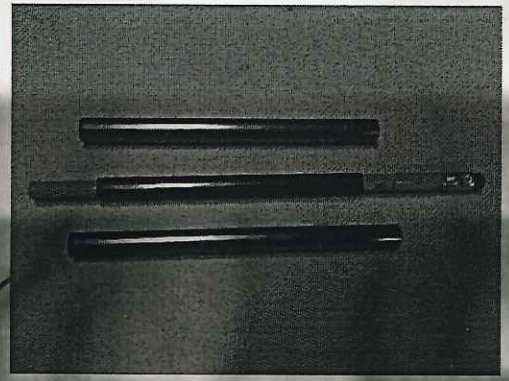

$H_2$ venting in emergency event



GE BWR Mark I

FIG 3





Fuel rods: Zr-alloy tube encasing Ur pellets

Zr oxidation:

$Zr + 2H_2O \rightarrow 2H_2 + ZrO_2$

Normal rate of deposition at low Temperatures: 10 microns / year.

Rate increases <u>dramatically</u> in the presence of water steam at high T in emergency events.

Exponential increase on $H_2$ carried by the steam

Table 2

Current $H_2/O_2$ reaction mechanism. The T range [K] corresponds to the published temperature range of the experimental validation for that reaction rate constant. $k = AT^n \exp(E_a/RT)$ in units of [s $^{-1}$], [cm$^3$mol $^{-1}$s $^{-1}$] or [cm$^6$mol $^{-2}$s $^{-1}$].

| No. | Reaction | A | n | $E_a$ [cal/mol] | Reference | Uncertainty (±%) | T range [K] |
|---|---|---|---|---|---|---|---|
| 1 | $H + O_2 = OH + O$ | 1.04E+14 | | 15,286 | [11] | 10 | 1100–3370 |
| 2 | $H + O_2 (+Ar) = HO_2 (+Ar)^a$ | 5.59E+13 | 0.2 | 0 | [43] | 18–35 | 1050–1250 |
| | Low-pressure limit | 6.81E+18 | 1.2 | 0 | [43] | – | – |
| | $H + O_2 (+H_2O) = HO_2 (+H_2O)^b$ | 5.59E+13 | 0.2 | 0 | [43] | – | – |
| | Low-pressure limit | 3.70E+19 | 1.0 | 0 | [43] | – | – |
| | $H + O_2 (+O_2) = HO_2 (+O_2)^c$ | 5.59E+13 | 0.2 | 0 | [43] | – | – |
| | Low-pressure limit | 5.69E+18 | 1.1 | 0 | [44] | – | – |
| | $H + O_2 (+M) = HO_2 (+M)^a$ | 5.59E+13 | 0.2 | 0 | [43] | – | – |
| | Low-pressure limit | 2.65E+19 | 1.3 | 0 | [43] | – | – |
| | Collider efficiency ($N_2 = 1$): $H_2 = 1.5$, $Ar = 0$, $H_2O = 0$, $O_2 = 0$ | | – | – | [44] | | |
| 3 | $H_2O_2 (+M) = 2OH (+M)^a$ | 8.59E+14 | | 48,560 | [14] | 21 | 1000–1200 |
| | Low-pressure limit | 9.55E+15 | | 42,203 | [12,16] | – | – |
| | Collider efficiency ($Ar = 1$): $N_2 = 1.5$, $H_2O = 9$ | | – | – | [12,59,60] | | |
| 4 | $OH + H_2O_2 = H_2O + HO_2$ | 1.74E+12 | | 318 | [16] | 27 | 1020–1460 |
| | $OH + H_2O_2 = H_2O + HO_2$ | 7.59E+13 | | 7269 | [16] | – | – |
| 5 | $OH + HO_2 = H_2O + O_2$ | 2.89E+13 | | 500 | [15] | 27 | 1600–2200 |
| 6 | $HO_2 + HO_2 = H_2O_2 + O_2$ | 1.30E+11 | | 1603 | [58] | | |
| | $HO_2 + HO_2 = H_2O_2 + O_2$ | 4.20E+14 | | 11,980 | [58] | | |
| 7 | $H_2O + M = H + OH + M$ | 6.06E+27 | 3.31 | 120,770 | [71] | | |
| | Collider efficiency ($Ar = 1$): $H_2O = 0$, $H_2 = 3$, $N_2 = 2$, $O_2 = 1.5$ | | | | [71] | | |
| | $H_2O + H_2O = OH + H + H_2O$ | 1.00E+26 | 2.44 | 120,160 | [71] | | |
| 8 | $OH + OH = H_2O + O$ | 3.57E+04 | 2.4 | 2111 | [74] | 15–25 | 1050–2380 |
| 9 | $O + H_2 = H + OH$ | 3.82E+12 | | 7948 | [45] | | |
| | $O + H_2 = H + OH$ | 8.79E+14 | | 19,170 | [45] | | |
| 10 | $H_2 + OH = H_2O + H$ | 2.17E+08 | 1.52 | 3457 | [45] | | |
| 11 | $H + HO_2 = OH + OH$ | 7.08E+13 | | 300 | [4] | | |
| 12 | $H + HO_2 = H_2O + O$ | 1.45E+12 | | 0 | [45] | | |
| 13 | $H + HO_2 = H_2 + O_2$ | 3.66E+06 | 2.087 | 1450 | [20] | | |
| 14 | $O + HO_2 = OH + O_2$ | 1.63E+13 | | 445 | [45] | | |
| 15 | $H_2O_2 + H = HO_2 + H_2$ | 1.21E+07 | 2.0 | 5200 | [18] | | |
| 16 | $H_2O_2 + H = H_2O + OH$ | 1.02E+13 | | 3577 | [45] | | |
| 17 | $H_2O_2 + O = OH + HO_2$ | 8.43E+11 | | 3970 | [45] | | |
| 18 | $H_2 + M = H + H + M$ | 5.84E+18 | 1.1 | 104,380 | [4] | | |
| | Collider efficiency ($Ar = 1$): $H_2O = 14.4$ | | | | [4,10] | | |
| | $H_2 + H_2 = H + H + H_2$ | 9.03E+14 | 0 | 96,070 | [45] | | |
| | $H_2 + N_2 = H + H + N_2$ | 4.58E+19 | 1.4 | 104,380 | [4] | | |
| | $H_2 + O_2 = H + H + O_2$ | 4.58E+19 | 1.4 | 104,380 | [4] | | |
| 19 | $O + O + M = O_2 + M$ | 6.16E+15 | 0.5 | 0 | [29] | | |
| | Collider efficiency ($N_2 = 1$): $H_2 = 2.5$, $H_2O = 12$, $Ar = 0$ | | | | [29] | | |
| | $O + O + Ar = O_2 + Ar$ | 1.89E+13 | 0 | 1788 | [29] | | |
| 20 | $O + H + M = OH + M$ | 4.71E+18 | 1.0 | 0 | [29] | | |
| | Collider efficiency ($N_2 = 1$): $H_2 = 2.5$, $H_2O = 12$, $Ar = 0.75$ | | | | [29] | | |

[a] $F_{cent} = 0.7$ [43].
[b] $F_{cent} = 0.8$ [43].
[c] $F_{cent} = 1$.

$H_2/O_2$ MECH (STANFORD)

9 SPECIES,

REMEASURED 6 RATES (1, 2, 3, 4, 5, 8)

BALANCE 1-10 DEFINES CROSSOVER TEMPERATURE.

| Reaction | | $A^a$ | $n^a$ | $E^a$ |
|---|---|---|---|---|
| **Hydrogen–oxygen chain** (SHUFFLE REACTIONS) | | | | |
| 1. $H + O_2 \rightleftarrows OH + O$ | R | $3.52\times10^{16}$ | -0.7 | 71.4 |
| 2. $H_2 + O \rightleftarrows OH + H$ | R | $5.06\times10^{4}$ | 2.7 | 26.3 |
| 3. $H_2 + OH \rightleftarrows H_2O + H$ | R | $1.17\times10^{9}$ | 1.3 | 15.2 |
| × 4. $H_2O + O \rightleftarrows OH + OH$ | | $7.60\times10^{0}$ | 3.8 | 53.4 |
| **Direct recombination** | | | | |
| 5.[b] $H + H + M \rightleftarrows H_2 + M$ | R | $1.30\times10^{18}$ | -1.0 | 0.0 |
| 6.[c] $H + OH + M \rightleftarrows H_2O + M$ | | $4.00\times10^{22}$ | -2.0 | 0.0 |
| × 7.[d] $O + O + M \rightleftarrows O_2 + M$ | | $6.17\times10^{15}$ | -0.5 | 0.0 |
| × 8.[e] $H + O + M \rightleftarrows OH + M$ | | $4.71\times10^{18}$ | -1.0 | 0.0 |
| × 9.[e] $O + OH + M \rightleftarrows HO_2 + M$ | | $8.00\times10^{15}$ | 0.0 | 0.0 |
| **Hydroperoxyl reactions** | | | | |
| 10.[f] $H + O_2 + M \rightleftarrows HO_2 + M$ | $k_0$ | $5.75\times10^{19}$ | -1.4 | 0.0 |
| | $k_\infty$ | $4.65\times10^{12}$ | 0.4 | 0.0 |
| 11. $HO_2 + H \rightleftarrows OH + OH$ | | $7.08\times10^{13}$ | 0.0 | 1.2 |
| 12. $HO_2 + H \rightleftarrows H_2 + O_2$ | R | $1.66\times10^{13}$ | 0.0 | 3.4 |
| × 13. $HO_2 + H \rightleftarrows H_2O + O$ | | $3.10\times10^{13}$ | 0.0 | 7.2 |
| × 14. $HO_2 + O \rightleftarrows OH + O_2$ | | $2.00\times10^{13}$ | 0.0 | 0.0 |
| 15. $HO_2 + OH \rightleftarrows H_2O + O_2$ | | $2.89\times10^{13}$ | 0.0 | -2.1 |
| **Hydrogen peroxide reactions** | | | | |
| 16.[g] $OH + OH + M \rightleftarrows H_2O_2 + M$ | $k_0$ | $2.30\times10^{18}$ | -0.9 | -7.1 |
| | $k_\infty$ | $7.40\times10^{13}$ | -0.4 | 0.0 |
| 17. $HO_2 + HO_2 \rightleftarrows H_2O_2 + O_2$ | | $3.02\times10^{12}$ | 0.0 | 5.8 |
| 18. $H_2O_2 + H \rightleftarrows HO_2 + H_2$ | | $4.79\times10^{13}$ | 0.0 | 33.3 |
| × 19. $H_2O_2 + H \rightleftarrows H_2O + OH$ | | $1.00\times10^{13}$ | 0.0 | 15.0 |
| × 20. $H_2O_2 + OH \rightleftarrows H_2O + HO_2$ | | $7.08\times10^{12}$ | 0.0 | 6.0 |
| × 21. $H_2O_2 + O \rightleftarrows HO_2 + OH$ | | $9.63\times10^{6}$ | 2.0 | 2.0 |

IN kJ / kg mol.

TABLE 1

MORE IMPORTANT THAN 10 IN RICH DEFLAGRATIONS

IGNORING THIS RESULTS IN BAD $\tau$ AND OH PROFILES IN LEAN DEFLAGRATIONS

CROSSOVER TEMPERATURE

INITIATION AT HIGH TEMPERATURES (←) IN DETONATIONS AND AUTOIGNITION

ALMOST ALWAYS NEGLIGIBLE.

MAIN TERMINATION. HEAT RELEASE

MAIN SOURCE OF $HO_2$

MAIN $HO_2$ REMOVAL

$[k] = \frac{cm^3}{mol\,s}$ BIMOLECULAR

$[k] = \frac{cm^6}{mol\,s}$ TRIMOLECULAR

$k_0$ → LOW-PRESSURE LIMIT

$k_\infty$ → HIGH-PRESSURE LIMIT

MAIN INITIATION STEP AT HIGH P AND LOW T (NEAR CROSSOVER). IMPORTANT ALSO FOR LEAN DEFLAGRATIONS NEAR THE FLAMMABILITY LIMIT.

INITIATION AT HIGH P AND LOW T (←)

AT HIGH PRESSURES AND LOW TEMPERATURES $[HO_2]$ IS LARGE AND GENERATES $H_2O_2$

[a] Specific reaction-rate constant $k = AT^n e^{-E/RoT}$ ; ~~units mol/cm³, s⁻¹, K, kJ/mol.~~

[b] Chaperon efficiencies are 2.5 for $H_2$, 12.0 for $H_2O$, 1.9 for CO, 3.8 for $CO_2$, 0.5 for Ar and He, and 1.0 for all other species.

[c] Chaperon efficiencies are 2.5 for $H_2$, 12.0 for $H_2O$, 1.9 for CO, 3.8 for $CO_2$, 0.4 for Ar and He, and 1.0 for all other species.

[d] Chaperon efficiencies are 2.5 for $H_2$, 12.0 for $H_2O$, 1.9 for CO, 3.8 for $CO_2$, 0.2 for Ar and He, and 1.0 for all other species.

[e] Chaperon efficiencies are 2.5 for $H_2$, 12.0 for $H_2O$, 1.9 for CO, 3.8 for $CO_2$, 0.7 for Ar and He, and 1.0 for all other species.

[f] Chaperon efficiencies are 2.5 for $H_2$, 16.0 for $H_2O$, 1.2 for CO, 2.4 for $CO_2$, 0.7 for Ar and He, and 1.0 for all other species; Troe falloff with $F_c = 0.5$.

[g] Chaperon efficiencies are 2.0 for $H_2$, 6.0 for $H_2O$, 1.5 for CO, 2.0 for $CO_2$, 0.4 for Ar and He, and 1.0 for all other species; Troe falloff with $F_c = 0.265 \exp(-T/94\text{ K}) + 0.735 \exp(-T/1756\text{ K}) + \exp(-5182\text{ K}/T)$.

CHAPERON EFFICIENCIES PREMULTIPLY A

CHAPERON EFFICIENCY FOR $N_2$ IS 1

GENERALLY, THEY DEPEND ON T BUT THE VARIATIONS ARE NOT THAT LARGE.

Table 1. The detailed mechanism and associated rate parameters.

$H_2/O_2$ MECHANISM (UCSD)

9 SPECIES ($H_2, O_2, H_2O, HO_2, OH, O, H, H_2O_2, M$)

(×) = FOR NONPREMIXED AND PREMIXED FLAMES, DETONATIONS AND AUTOIGNITION IN PRACTICAL CONDITIONS,

FIG 4

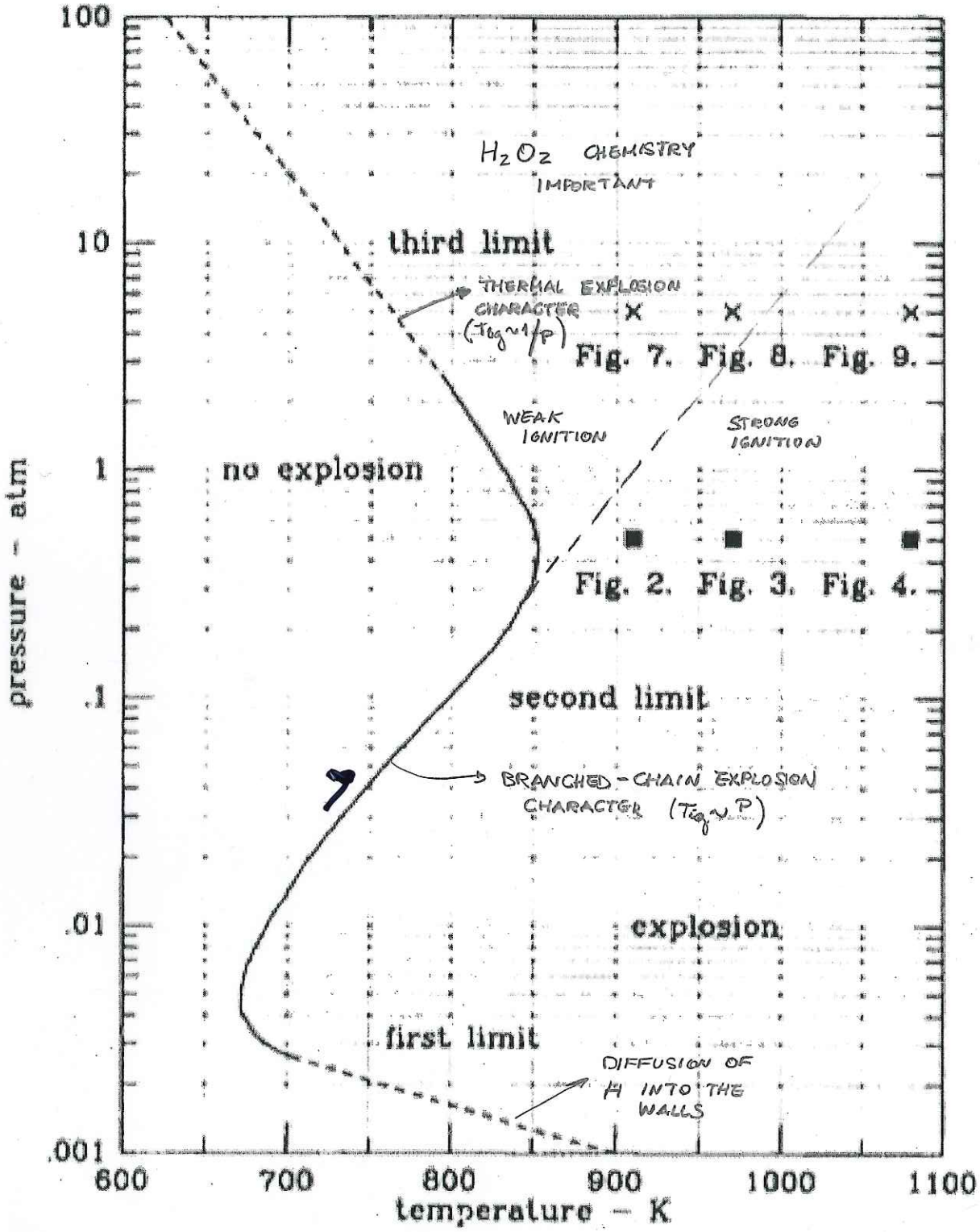



**Figure 1.** Explosion limits for a stoichiometric mixture of hydrogen and oxygen (from [32]). The dashed lines are extrapolations of the first and third limits. The symbols

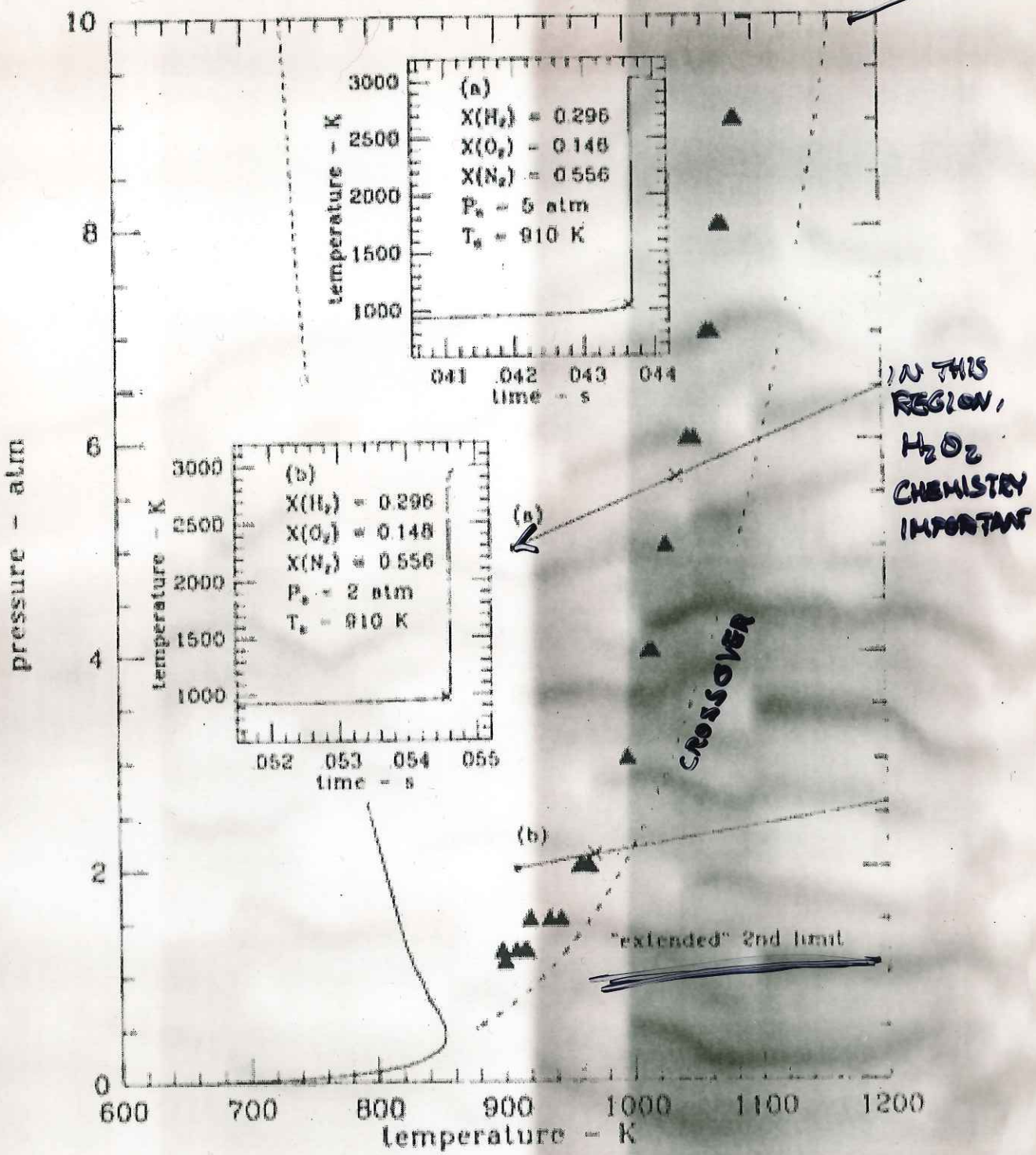



Figure 12. Explosion limits for stoichiometric mixtures of hydrogen and oxygen. The solid line in the lower left hand corner of the figure and the dashed line are the second and third explosion limits shown earlier in Figure 1. The dash-dot-dash line is the classical "extended" second limit. The solid triangles are the transition temperatures calculated from the eigenanalysis of the kinetic solutions for the dilute mixture consisting of 1% $H_2$, 0.5% $O_2$, and 98.5% $N_2$. The two insert figures report the temperature profiles

$H_2/O_2$ AUTOIGNITION TIME

FIG 7

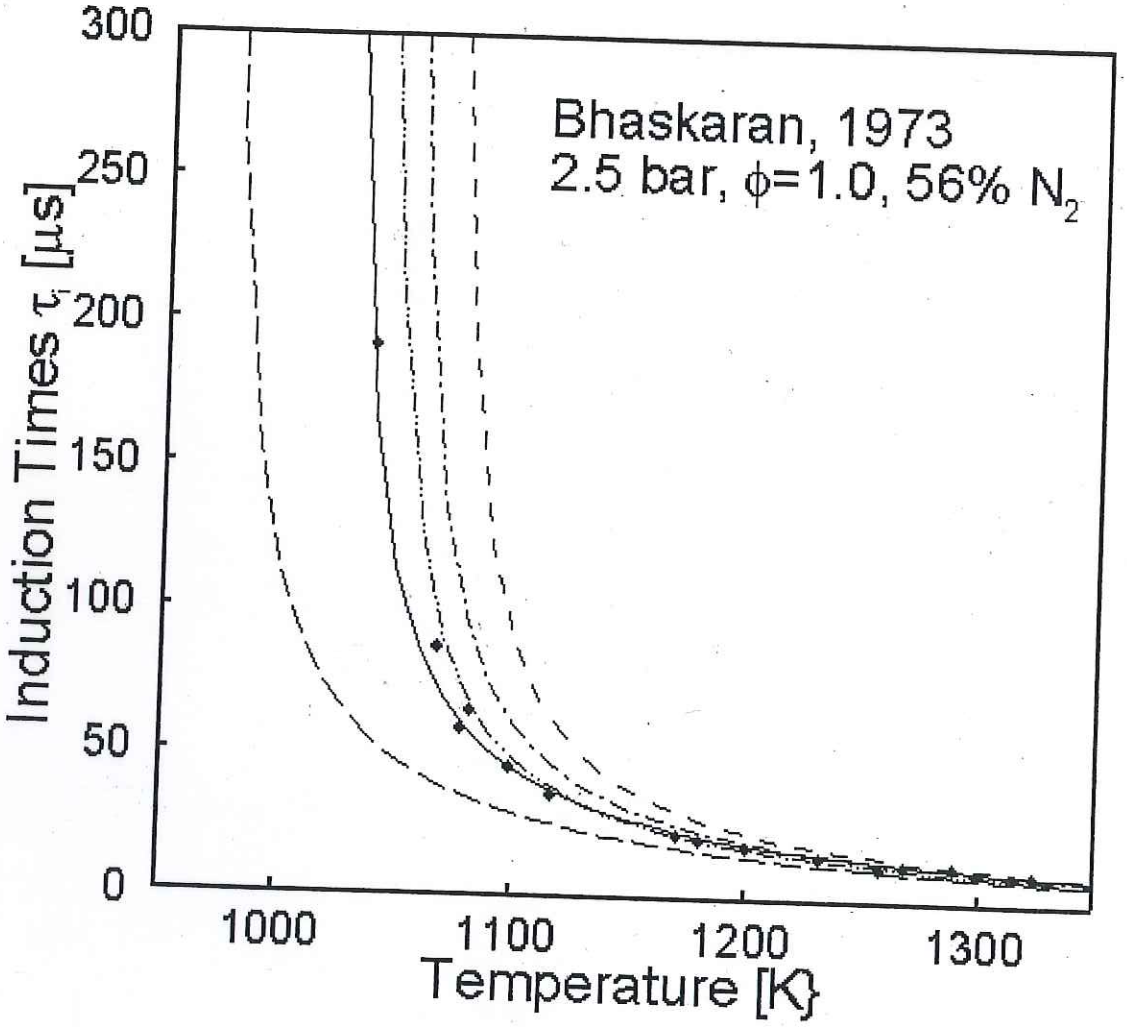
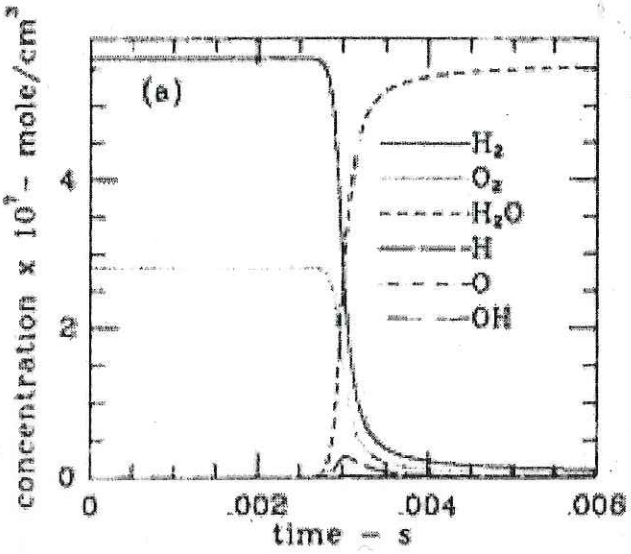


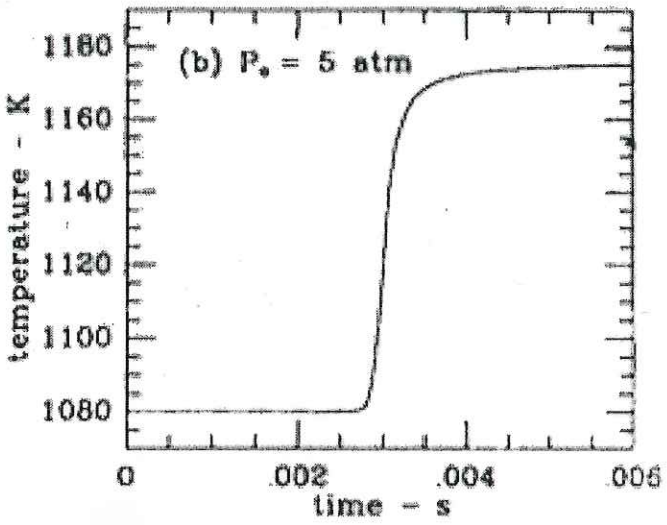

Figure 6. Variation with temperature of the induction time as obtained from detailed-chemistry numerical calculations (solid curve [23], short-dashed curve [11], long-dashed curve [20], dot-dashed curve [15], dot-dot-dashed curve [18]) and from shock-tube experimental results [54] (p = 2.5 bar, $\phi$ = 1, solid points).

FIG 8

YETTER ET AL (1991)

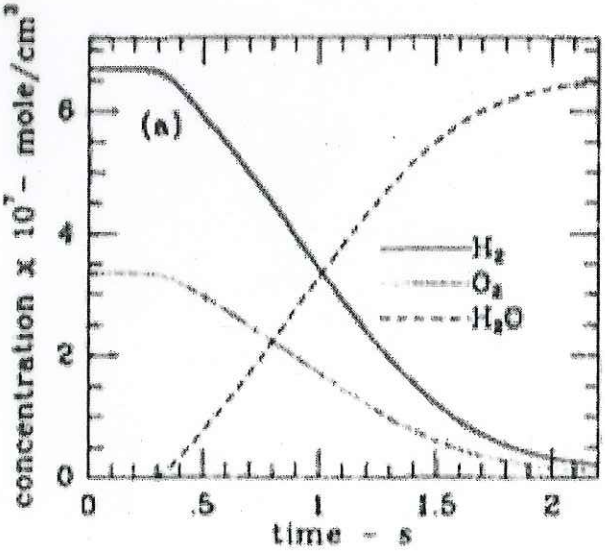
T=1080K

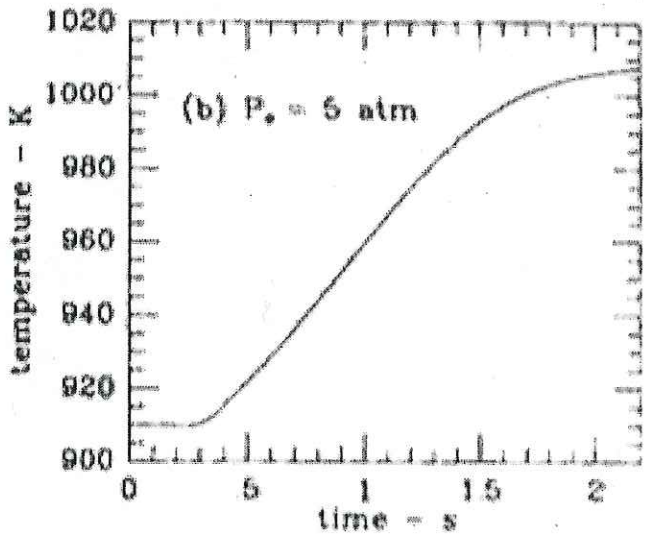



WC STRONG AUTOIGNITION

T=910 K




WEAK AUTOIGNITION

FIG 9a

5-STEP CHEMISTRY FOR $H_2/O_2$ AUTOIGNITION (DEL ALAMO ET AL, 2006)

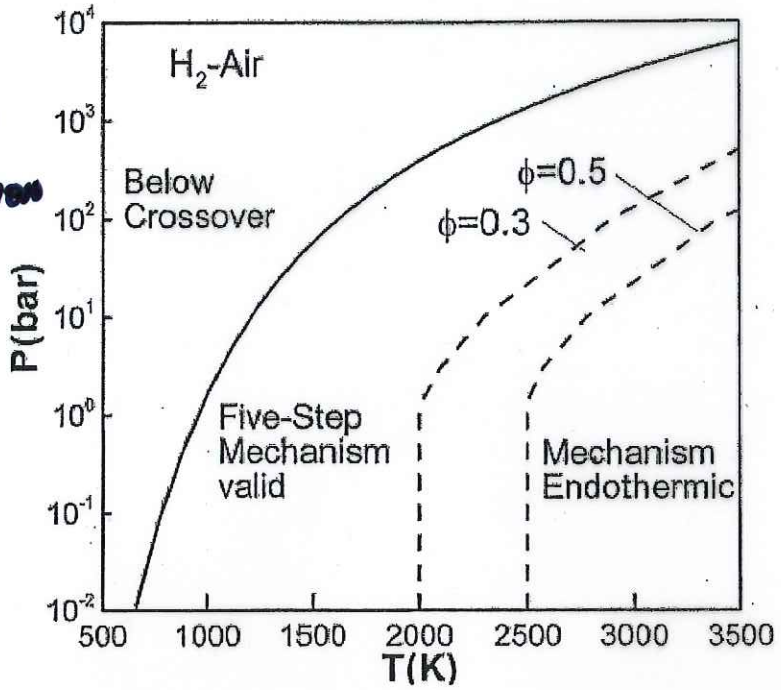



Figure 12. Estimated region of validity, in a pressure-temperature plane, for autoignition-time predictions by the five-step mechanism for hydrogen-air mixtures.

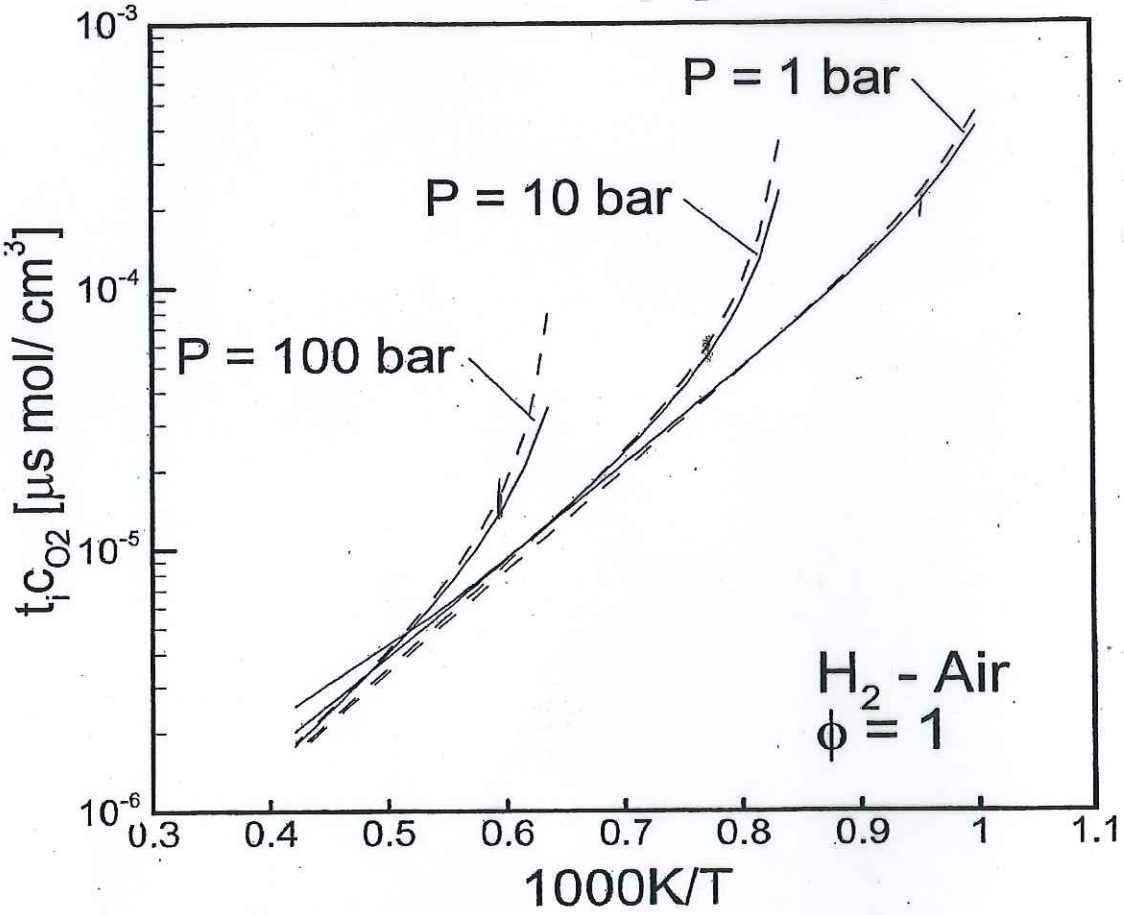
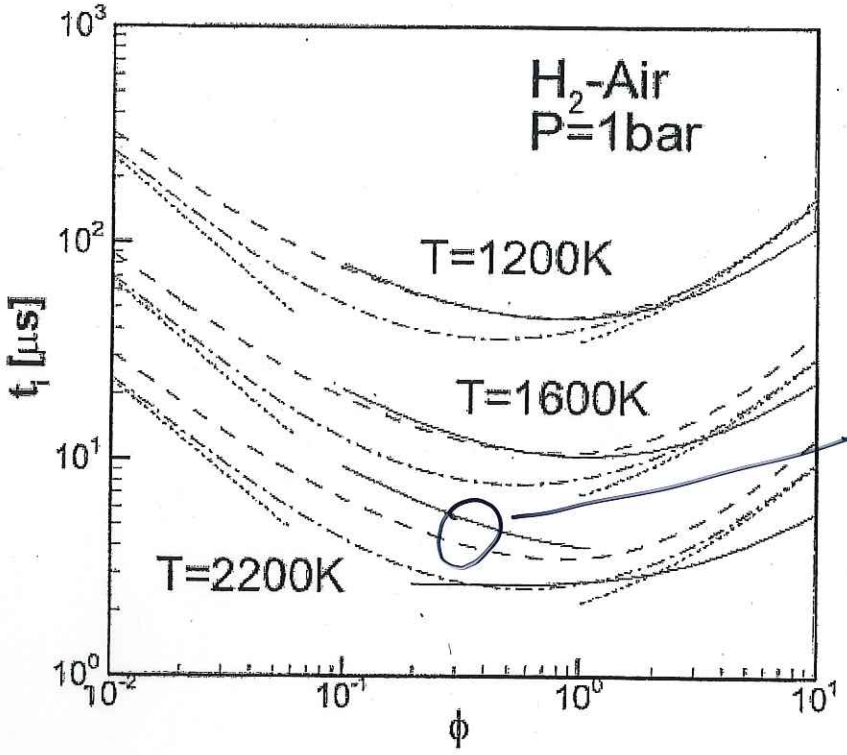



Figure 11. The temperature dependence of the product of the ignition time and the oxygen concentration for stoichiometric hydrogen-air mixtures at three different pressures according to the temperature-inflection criterion, for the detailed mechanism of Table 1 (solid curves) and for the reduced mechanism of Table 3 (dashed curves).

FIG 9b




-.-.- 5-STEP

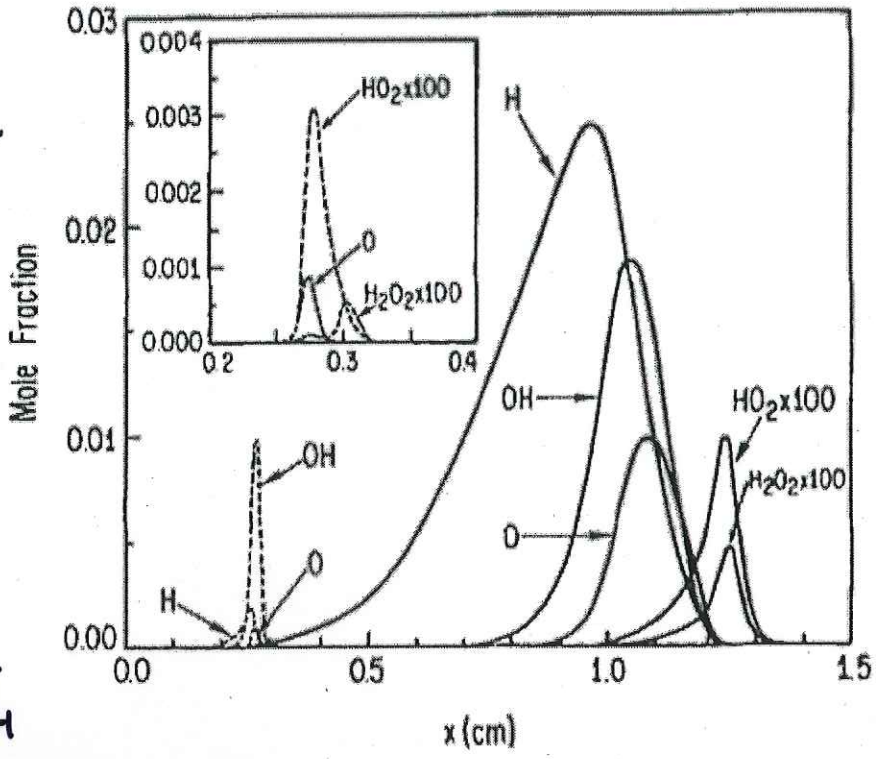
- - - - 21-STEP

AT HIGH T THE IGNITION CRITERION MATTERS

Figure 13. Hydrogen-air autoignition times as functions of the equivalence ratio at 1 bar for three different temperatures according to Eqs. 44 and 45 (dotted lines), eq. 46 (dot-dash curves), numerical integration of the detailed mechanism under isothermal conditions with achievement of 95% of partial equilibrium of $H + O_2 \rightarrow OH + O$ as the ignition criterion (dashed curves) and numerical integrations of the detailed mechanism under adiabatic conditions with temperature inflection as the ignition criterion (solid curves).

GUTHEIL + WILLIAMS (1990)

$H_2$ / AIR DIFFUSION FLAMES



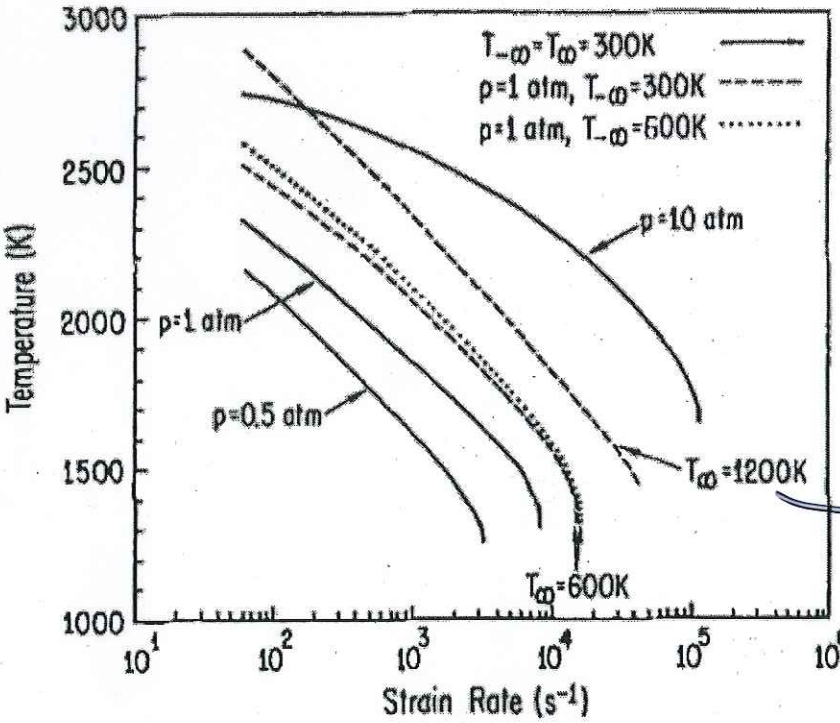

↑P ↓$\delta_f$
↑P ↑$T_f$
↑P ↑$X_i$ EXCEPT FOR OH

FIG. 5. Profiles of $X_i$ for minor species at $a = 60$ $s^{-1}$ and $T_{-\infty} = T_\infty = 300$ K, for $p = 0.5$ atm (solid curves) and for $p = 10$ atm (dashed curves).

FIG 10b

↑P ↑$a_{EXT}$

10-FOLD INCREASE ON P → $10^3$-FOLD INCREASE ON $a_{EXT}$




↑P ↑$T_f$ CONSISTENT WITH 2ND EXPLOSION LIMIT

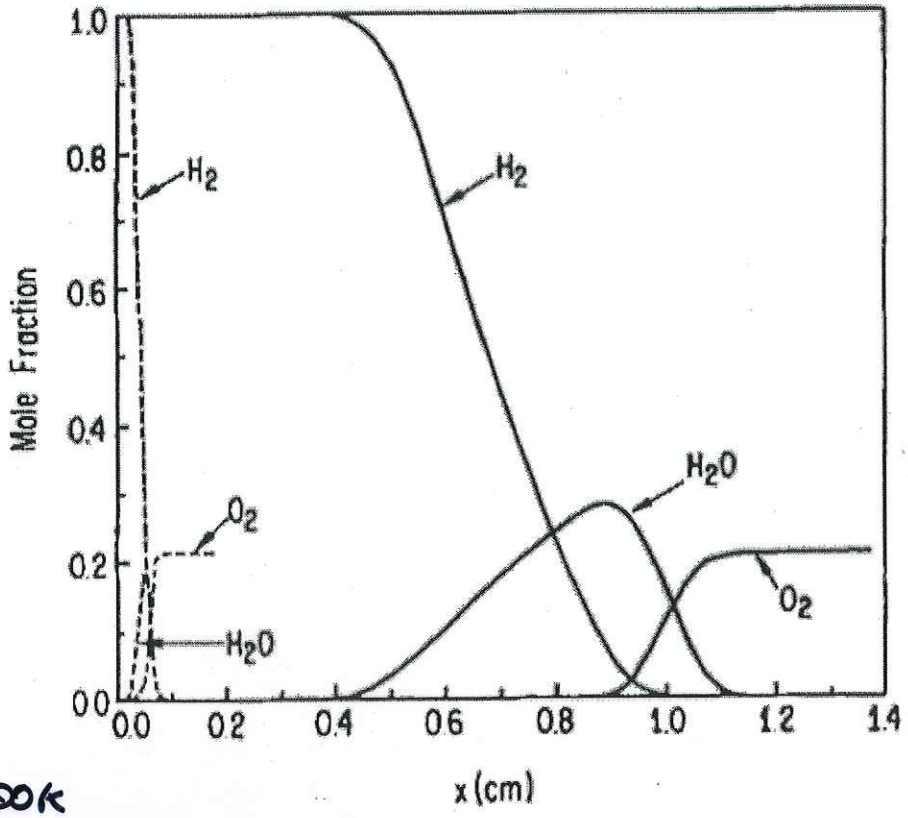
FOR T > 1200K THERE IS NO EXTINCTION AT P = 1 ATM. ($T_\infty > T_c$)

CROSSOVER

FIG. 6. The dependence of the maximum temperature on the strain rate for various pressures and ambient temperatures.

$H_2$/AIR DIFFUSION FLAMES

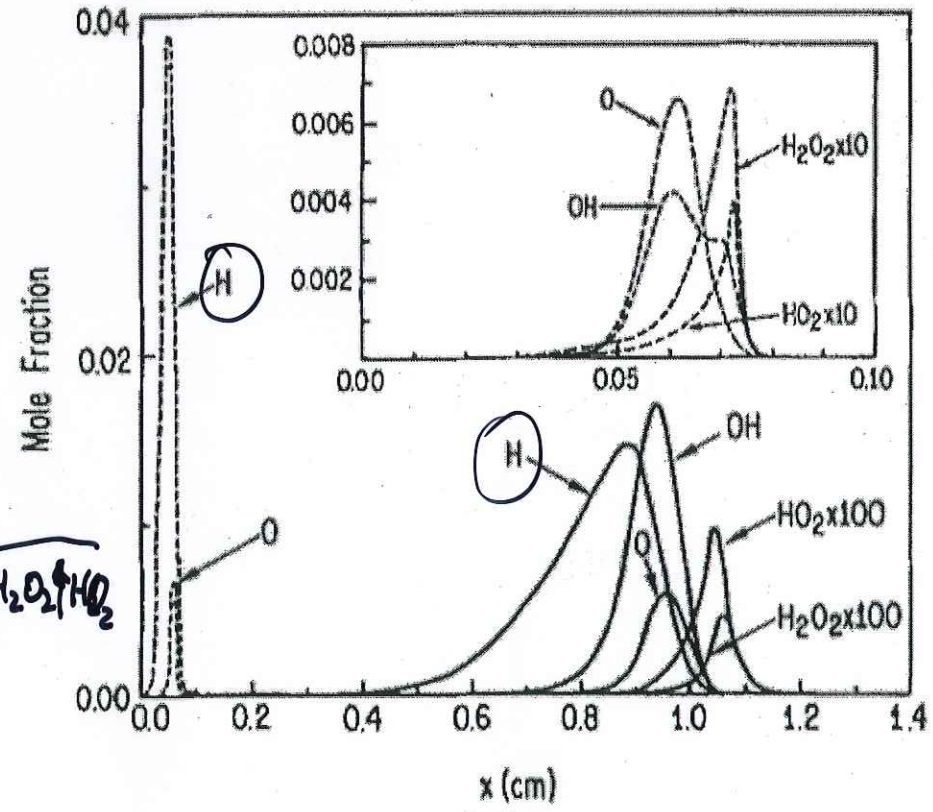
GUTHEIL + WILLIAMS (1990)




$a_{EXT} \sim 8140\ s^{-1}$
AT P = 1 ATH
$T_\infty = T_{-\infty} = 300K$

FIG. 2. Profiles of $X_i$ for major species at $p = 1$ atm and $T_{-\infty} = T_\infty = 300$ K, for $a = 60\ s^{-1}$ (solid curves) and for $a = 8000\ s^{-1}$ (dashed curves).

FIG 10a




$X_i$
$\uparrow a$ $\uparrow H$ $\downarrow OH$ $\uparrow H_2O_2 \uparrow HO_2$

FIG. 3. Profiles of $X_i$ for minor species at $p = 1$ atm and $T_{-\infty} = T_\infty = 300$ K, for $a = 60\ s^{-1}$ (solid curves) and for $a = 8000\ s^{-1}$ (dashed curves).

FIG 11

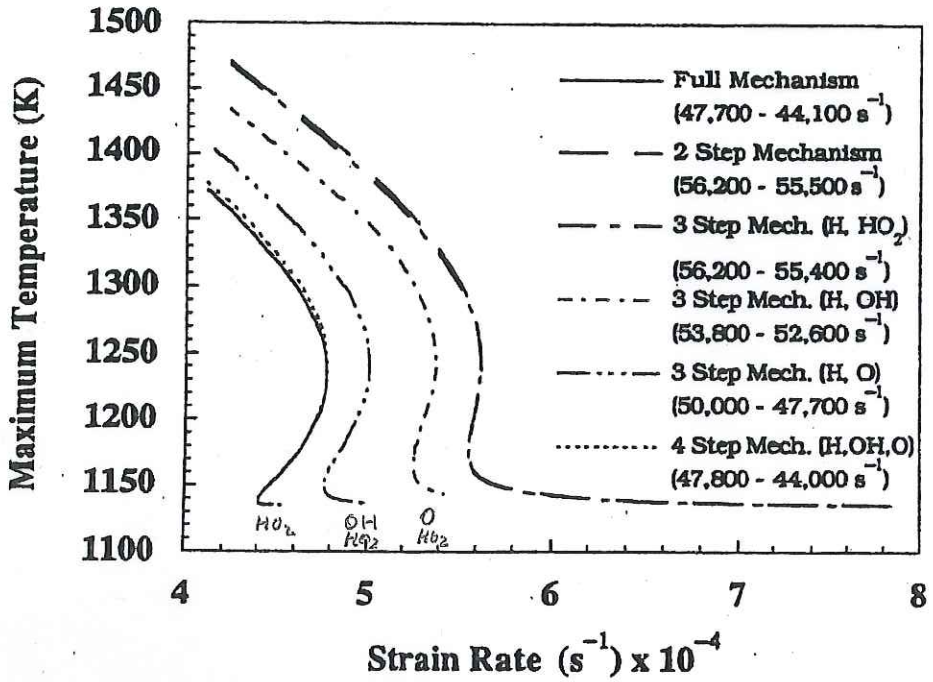



Figure 18. The maximum calculated temperature in the diffusion flame, as a function of the air-side strain rate, for a steady, axisymmetric counterflow flame between air at 1135 K and a molar mixture of 40% hydrogen and 60% nitrogen, according to the full mechanism of Table 1, the four-step mechanism of Eq. 54, the three-step mechanisms of Eqs. 64, 60 and 69, and the two-step mechanism of Eqs. 31 and 53.



$H_2$-$O_2$ DIFFUSION FLAMES

(WILLIAMS, UNPUBLISHED)

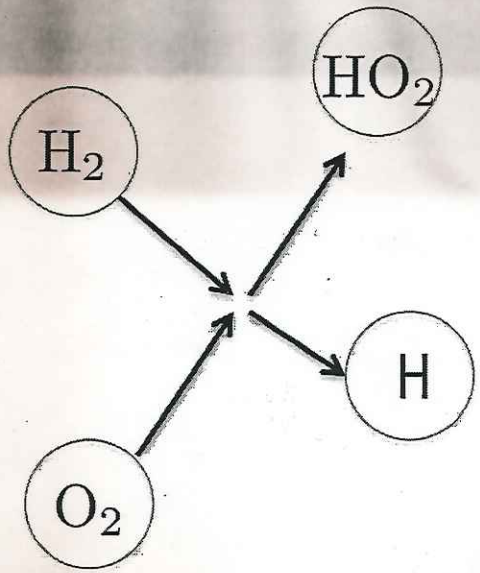
BRACKETS INDICATE SPECIES ASSUMED TO BE OUT OF STEADY STATE.

ONLY ABOUT CROSSOVER!

# The initiation - branching – termination

## Initiation

$$H_2 + O_2 \overset{12}{\rightleftharpoons} HO_2 + H$$




SLOW TIMESCALE

$t_I$

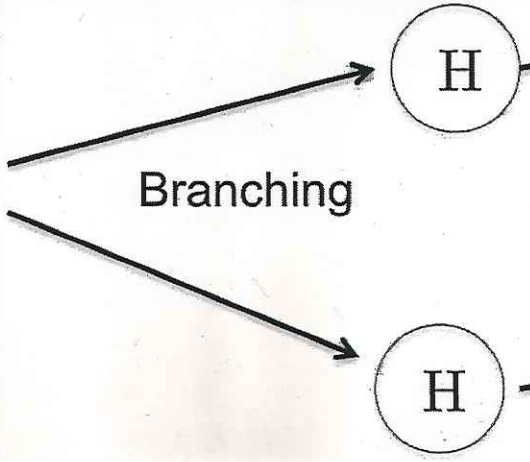
## Branching

$$H + O_2 \overset{1}{\rightleftharpoons} OH + O$$

$$H_2 + O \overset{2}{\rightleftharpoons} OH + H$$

$$H_2 + OH \overset{3}{\rightleftharpoons} H_2O + H$$

Controlled by 1 when O and OH are in SS

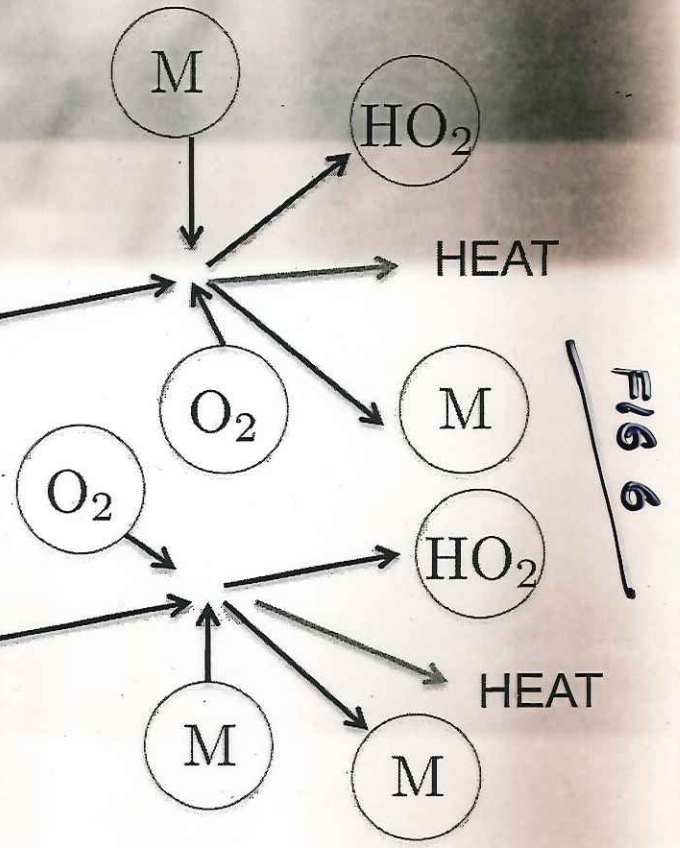



FAST ($T>T_c$) / SLOW ($T<T_c$) TIMESCALE

$t_B$

## Termination

$$H + O_2 + M \overset{10}{\rightleftharpoons} HO_2 + M$$




FAST ($T<T_c$) / SLOW ($T>T_c$) TIMESCALE

$t_T$

Fig 6

FIG 12

(BOLVIN ET AL, 2010)

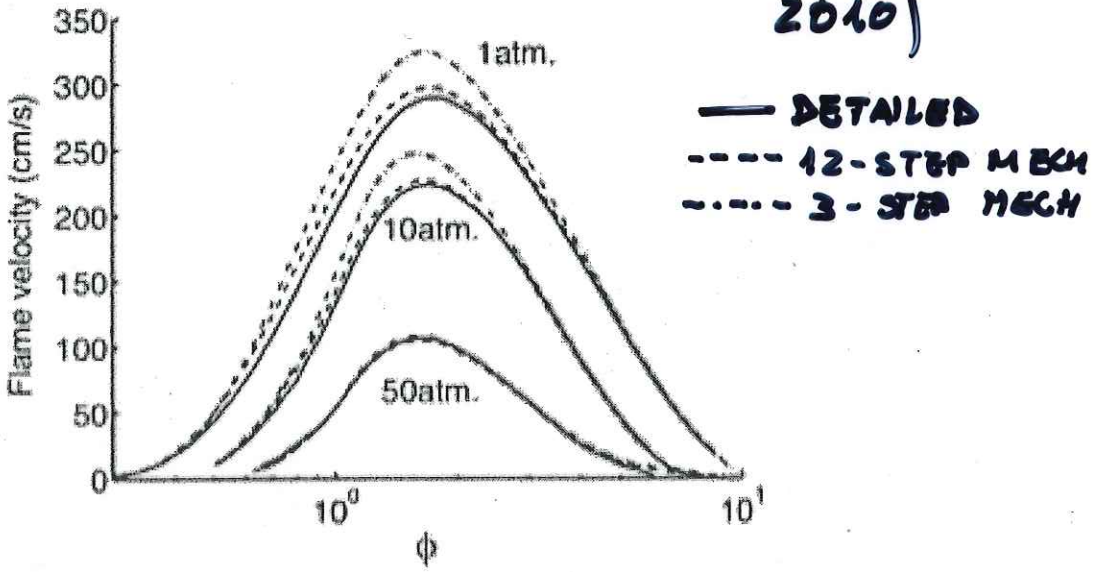



Fig. 1. The variation with equivalence ratio of the laminar burning rate of hydrogen–air planar deflagrations with initial temperature $T_u = 300$ K and three different pressures as obtained with the detailed 21-step chemistry (solid curves), with the short 12-step chemistry (dashed curves) and with the 3-step reduced mechanism (dot-dashed curves).

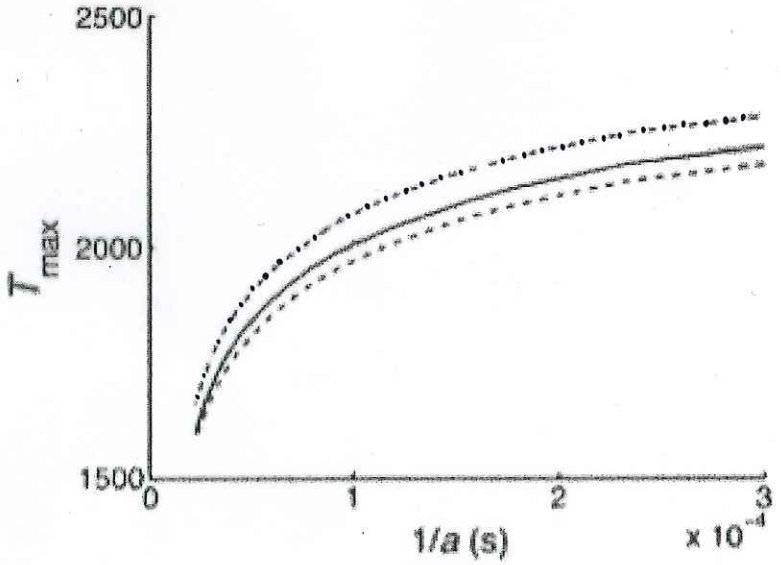



Fig. 2. The variation with strain rate of the maximum temperature in a hydrogen–air planar counterflow at atmospheric pressure with feed-stream temperatures $T = 300$ K as obtained with the detailed 21-step chemistry (solid curves), with the short 12-step chemistry (dashed curves) and with the 3-step reduced mechanism (dot-dashed curves).

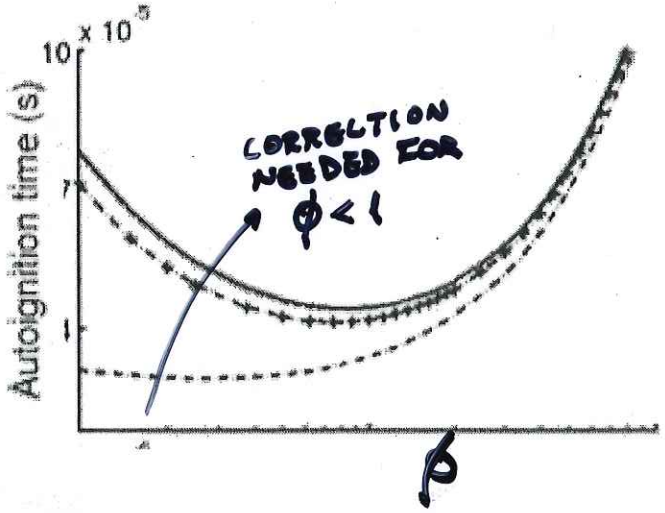



Fig. 3. The variation with equivalence ratio of the induction time in isobaric homogeneous combustion for different conditions of pressure and initial temperature (upper plot: $T = 1200$ K and $p = 1$ atm; middle plot: $T = 1500$ K and $p = 10$ atm; lower plot: $T = 1800$ K and $p = 50$ atm) as obtained with the detailed 21-step chemistry (solid curves), with the short 12-step chemistry (dashed curves) and with the 3-step reduced mechanism (dot-dashed curves), with the crosses indicating the results obtained with the modified reaction rates (9).

CH4-O2 MECH.

TABLE 3

The Elementary Reaction Mechanism and Associated Rate Coefficients

| No. | Reaction | $B^a$ | $\alpha^a$ | $E^a$ $(=RT_a)$ |
|---|---|---|---|---|
| *1* | $O_2 + H \rightarrow OH + O$ | $2.00 \times 10^{14}$ | 0.00 | 70.30 |
| *1b* | $OH + O \rightarrow O_2 + H$ | $1.40 \times 10^{13}$ | 0.00 | 3.20 |
| *2* | $O + H_2 \rightarrow H + OH$ | $1.50 \times 10^{7}$ | 2.00 | 31.60 |
| *2b* | $H + OH \rightarrow O + H_2$ | $6.73 \times 10^{6}$ | 2.00 | 22.35 |
| *3* | $OH + H_2 \rightarrow H + H_2O$ | $1.00 \times 10^{8}$ | 1.60 | 13.80 |
| *3b* | $H + H_2O \rightarrow OH + H_2$ | $4.62 \times 10^{8}$ | 1.60 | 77.50 |
| 4 | $OH + OH \rightarrow H_2O + O$ | $1.50 \times 10^{9}$ | 1.14 | 0.42 |
| 4b | $H_2O + O \rightarrow OH + OH$ | $1.49 \times 10^{10}$ | 1.14 | 71.14 |
| *5*[b] | $H + O_2 + M \rightarrow OH_2 + M$ | $2.30 \times 10^{18}$ | −0.80 | 0.00 |
| 6 | $HO_2 + H \rightarrow OH + OH$ | $1.50 \times 10^{14}$ | 0.00 | 4.20 |
| 7 | $HO_2 + H \rightarrow H_2 + O_2$ | $2.50 \times 10^{13}$ | 0.00 | 2.90 |
| 8 | $HO_2 + H \rightarrow H_2O + O$ | $3.00 \times 10^{13}$ | 0.00 | 7.20 |
| 9 | $HO_2 + OH \rightarrow H_2O + O_2$ | $6.00 \times 10^{13}$ | 0.00 | 0.00 |
| *10* | $CO + OH \rightarrow CO_2 + H$ | $4.40 \times 10^{6}$ | 1.50 | −3.10 |
| *10b* | $CO_2 + H \rightarrow CO + OH$ | $4.96 \times 10^{8}$ | 1.50 | 89.71 |
| *11* | $CH_4 + H \rightarrow H_2 + CH_3$ | $2.20 \times 10^{4}$ | 3.00 | 36.60 |
| 11b | $H_2 + CH_3 \rightarrow CH_4 + H$ | $8.83 \times 10^{2}$ | 3.00 | 33.53 |
| 12 | $CH_4 + OH \rightarrow H_2O + CH_3$ | $1.60 \times 10^{6}$ | 2.10 | 10.30 |
| *13* | $CH_3 + O \rightarrow CH_2O + H$ | $7.00 \times 10^{13}$ | 0.00 | 0.00 |
| 14 | $CH_3 + OH \rightarrow CH_2O + H + H$ | $9.00 \times 10^{14}$ | 0.00 | 64.80 |
| 15 | $CH_3 + OH \rightarrow CH_2O + H_2$ | $8.00 \times 10^{12}$ | 0.00 | 0.00 |
| 16[c] | $CH_3 + H \rightarrow CH_4$ | $6.00 \times 10^{16}$ | −1.00 | 0.00 |
| *17* | $CH_2O + H \rightarrow CHO + H_2$ | $2.50 \times 10^{13}$ | 0.00 | 16.70 |
| 18 | $CH_2O + OH \rightarrow CHO + H_2O$ | $3.00 \times 10^{13}$ | 0.00 | 5.00 |
| 19 | $CHO + H \rightarrow CO + H_2$ | $2.00 \times 10^{14}$ | 0.00 | 0.00 |
| 20 | $CHO + OH \rightarrow CO + H_2O$ | $1.00 \times 10^{14}$ | 0.00 | 0.00 |
| 21 | $CHO + O_2 \rightarrow CO + HO_2$ | $3.00 \times 10^{12}$ | 0.00 | 0.00 |
| *22*[b] | $CHO + M \rightarrow CO + H + M$ | $7.10 \times 10^{14}$ | 0.00 | 70.30 |
| 23 | $CH_3 + H \rightarrow CH_2 + H_2$ | $1.80 \times 10^{14}$ | 0.00 | 63.00 |
| 24 | $CH_2 + O_2 \rightarrow CO_2 + H + H$ | $6.50 \times 10^{12}$ | 0.00 | 6.30 |
| 25 | $CH_2 + O_2 \rightarrow CO + OH + H$ | $6.50 \times 10^{12}$ | 0.00 | 6.30 |
| 26 | $CH_2 + H \rightarrow CH + H_2$ | $4.00 \times 10^{13}$ | 0.00 | 0.00 |
| 26b | $CH + H_2 \rightarrow CH_2 + H$ | $2.79 \times 10^{13}$ | 0.00 | 12.61 |
| 27 | $CH + O_2 \rightarrow CHO + O$ | $3.00 \times 10^{13}$ | 0.00 | 0.00 |
| 28 | $CH_3 + OH \rightarrow CH_2 + H_2O$ | $1.50 \times 10^{13}$ | 0.00 | 20.93 |
| 29 | $CH_2 + OH \rightarrow CH_2O + H$ | $2.50 \times 10^{13}$ | 0.00 | 0.00 |
| 30 | $CH_2 + OH \rightarrow CH + H_2O$ | $4.50 \times 10^{13}$ | 0.00 | 12.56 |
| 31 | $CH + OH \rightarrow CHO + H$ | $3.00 \times 10^{13}$ | 0.00 | 0.00 |

[a] Here cm, mol, K, and kJ are the units, with the notation of Eq. (14).

[b] Catalytic efficiencies were taken from [1].

[c] The high-pressure value $k_\infty$ is given here; tail-off curves, $k/k_\infty = (1 + 21.5 \times 10^{10} T^3/p^{0.6})^{-1}$, where $p$ is in atm and $T$ in K, were approximated from Fig. 30 in [1].

PETERS AND WILLIAMS (1987)

→ 4-STEP MECHANISM:

I. $CH_4 + 2H + H_2O \rightarrow CO + 4H_2$ TERM

II. $CO + H_2O \rightleftharpoons CO_2 + H_2$ CO OX

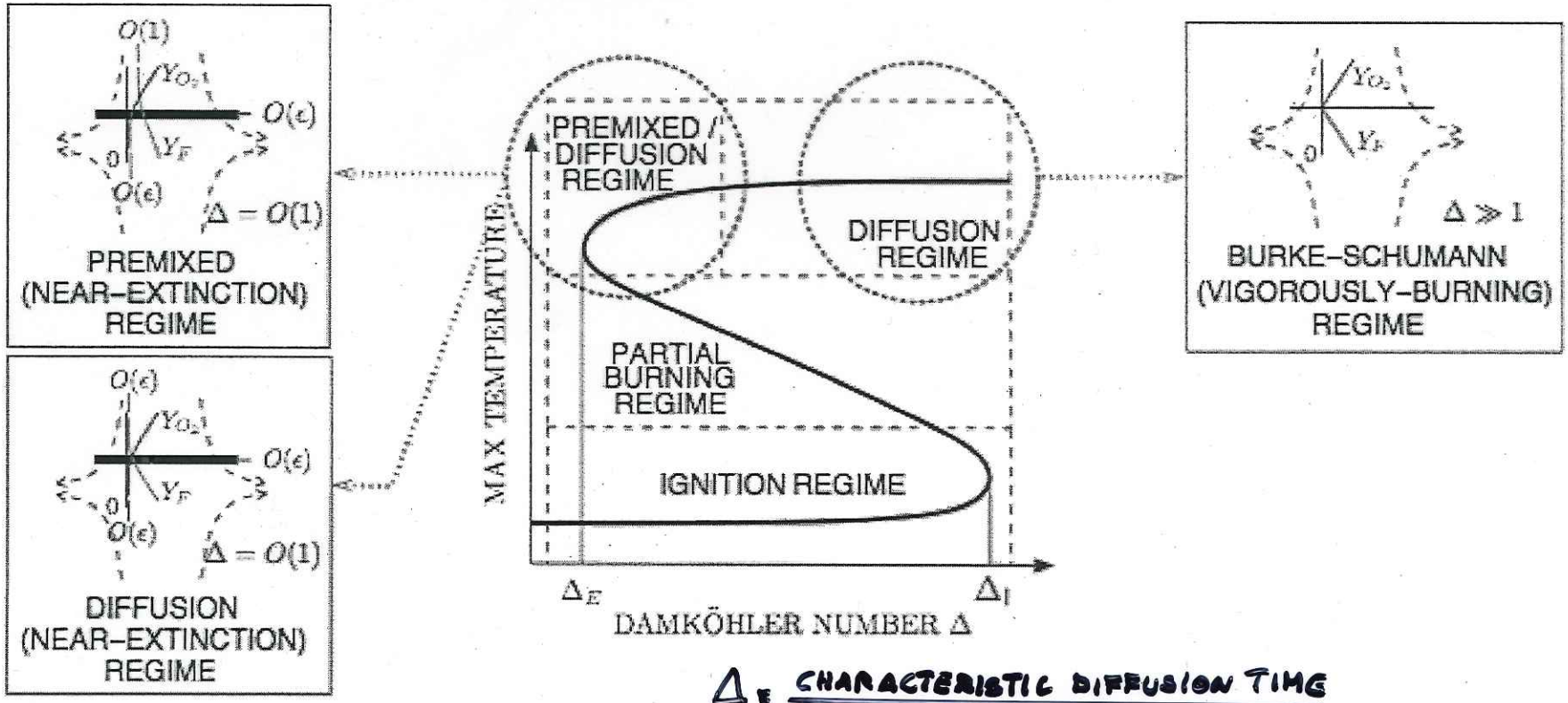
III. $H + H + M \rightleftharpoons H_2 + M$ TERM

IV. $O_2 + 3H_2 \rightleftharpoons 2H + 2H_2O$ BRANCH.

WITH

(17)

(17)



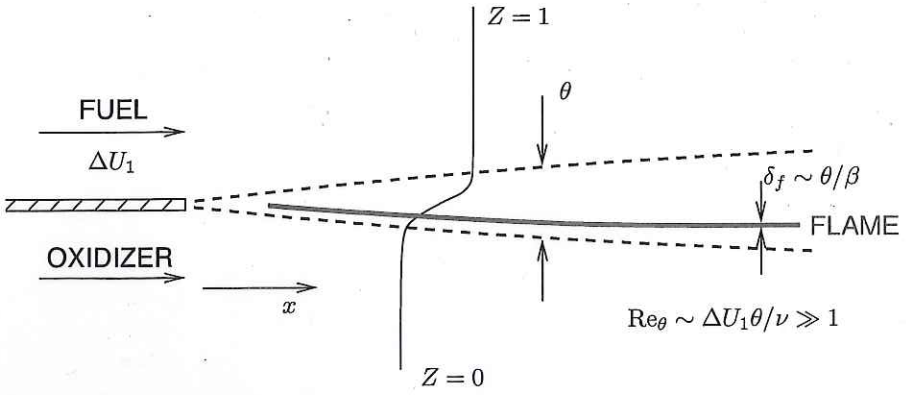

$\Delta$ = CHARACTERISTIC DIFFUSION TIME / LOCAL CHEMICAL TIME

Figure 3.1: Liñán [23] S-curve, asymptotic orderings and burning regimes schematics.

FIG 13: S-CURVE FOR DIFFUSION FLAMES

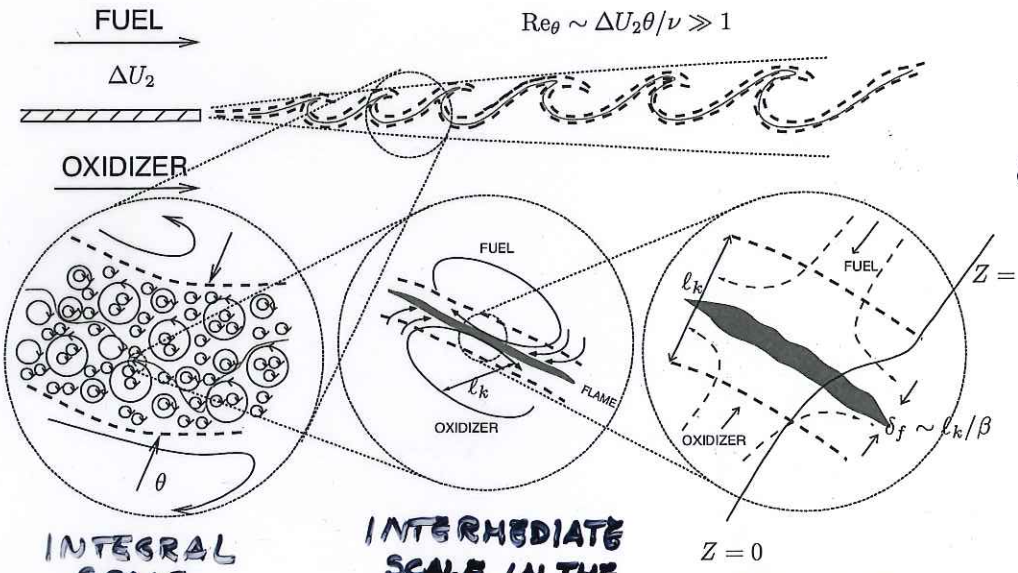
FIG 14

# " THE TURBULENT-COMBUSTION PROBLEMATIQUE "




LAMINAR MIXING LAYER

$t_d^L \sim \theta^2/D_F$ DIFFUSION TIME THROUGH MIXING LAYER




TURBULENT MIXING LAYER

KOLMOGOROV TIME

$t_d^T \sim \ell_k^2/D_F \sim t_d^L \mathrm{Re}_\theta^{-1/2} \ll t_d^L$

$t_l \sim \theta/\Delta U_2 \gg t_d^T \gg t_c^T$

INTEGRAL TIME

INTEGRAL SCALE

$L \sim \Theta$

INTERMEDIATE SCALE IN THE INERTIAL SUBRANGE

$\Theta > L > \ell_k$

KOLMOGOROV SCALES

$L \leq \ell_k$

TURBULENT DIFFUSIVITY $D_T$

$$\frac{\Theta \Delta U}{D_T} \sim 1$$

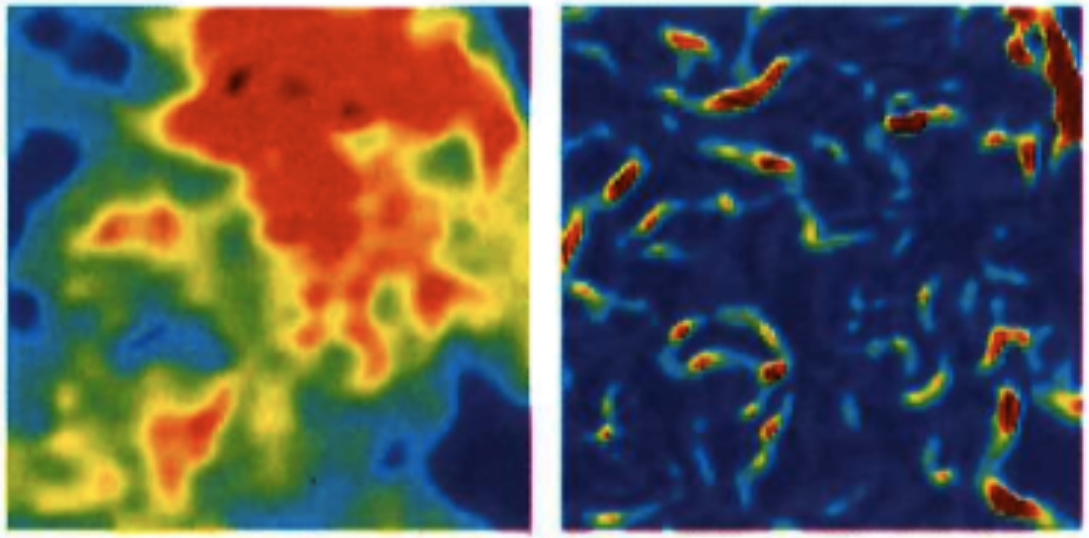
WITH $\frac{1}{D_T} \sim \frac{1}{\mathrm{Re}_\Theta} \ll 1$

RANS → LES → DNS

NOTE THAT, AT THIS LEVEL: $D|\partial Z|^2 \to$ FINITE NUMBER AS $D \to 0$ ($\mathrm{Re} \to \infty$)

NOTE: FOR DNS IN COMBUSTION, $L < \delta_f$ NOT DNS OTHERWISE!

# SCALAR DISSIPATION RATE



(a) (b)

Fig. 3.8 (a) Instantaneous close-up of a 2-D mixture fraction measurement in a turbulent air plume and (b) the associated scalar dissipation. The image shown is 100×100 pixels, with 1 pixel corresponding to about 0.060 mm. Red corresponds to high values, blue to zero. Data courtesy of Dr. C.N. Markides.

# DNS

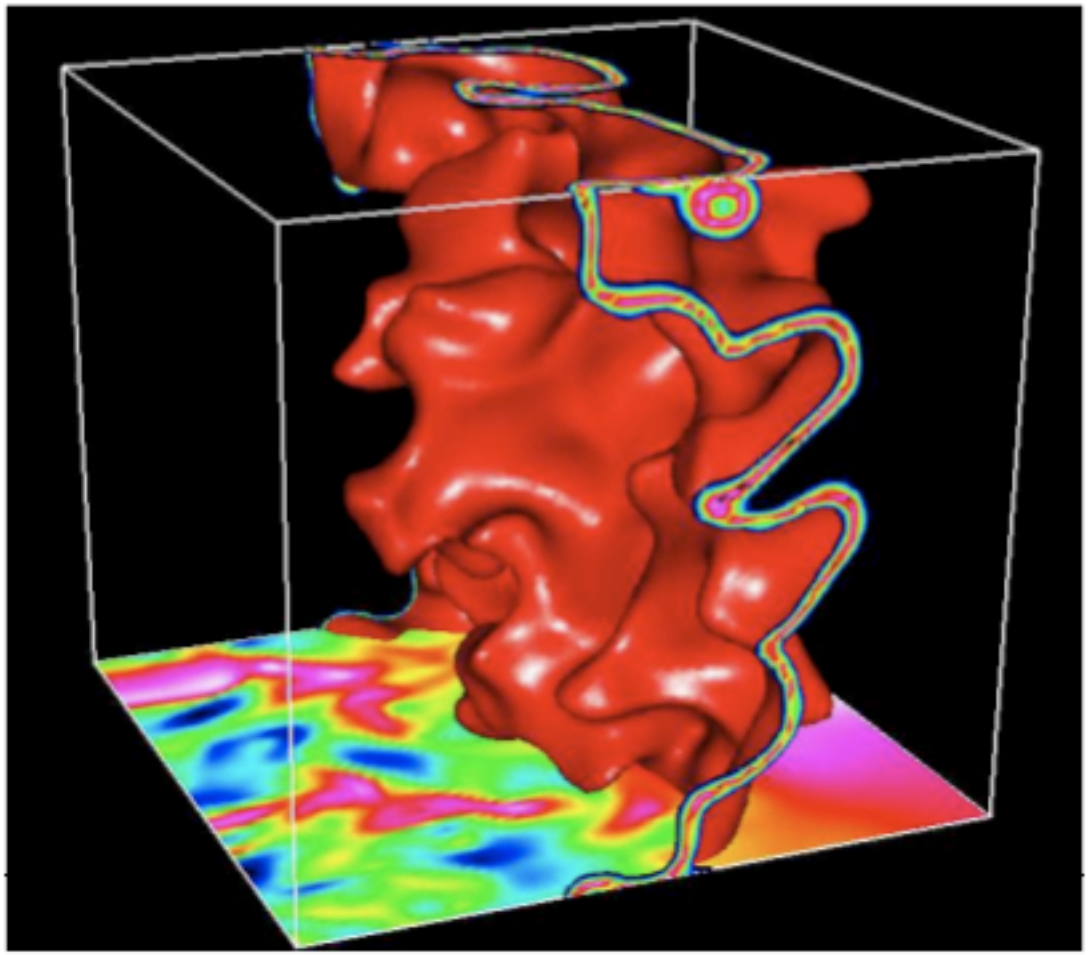
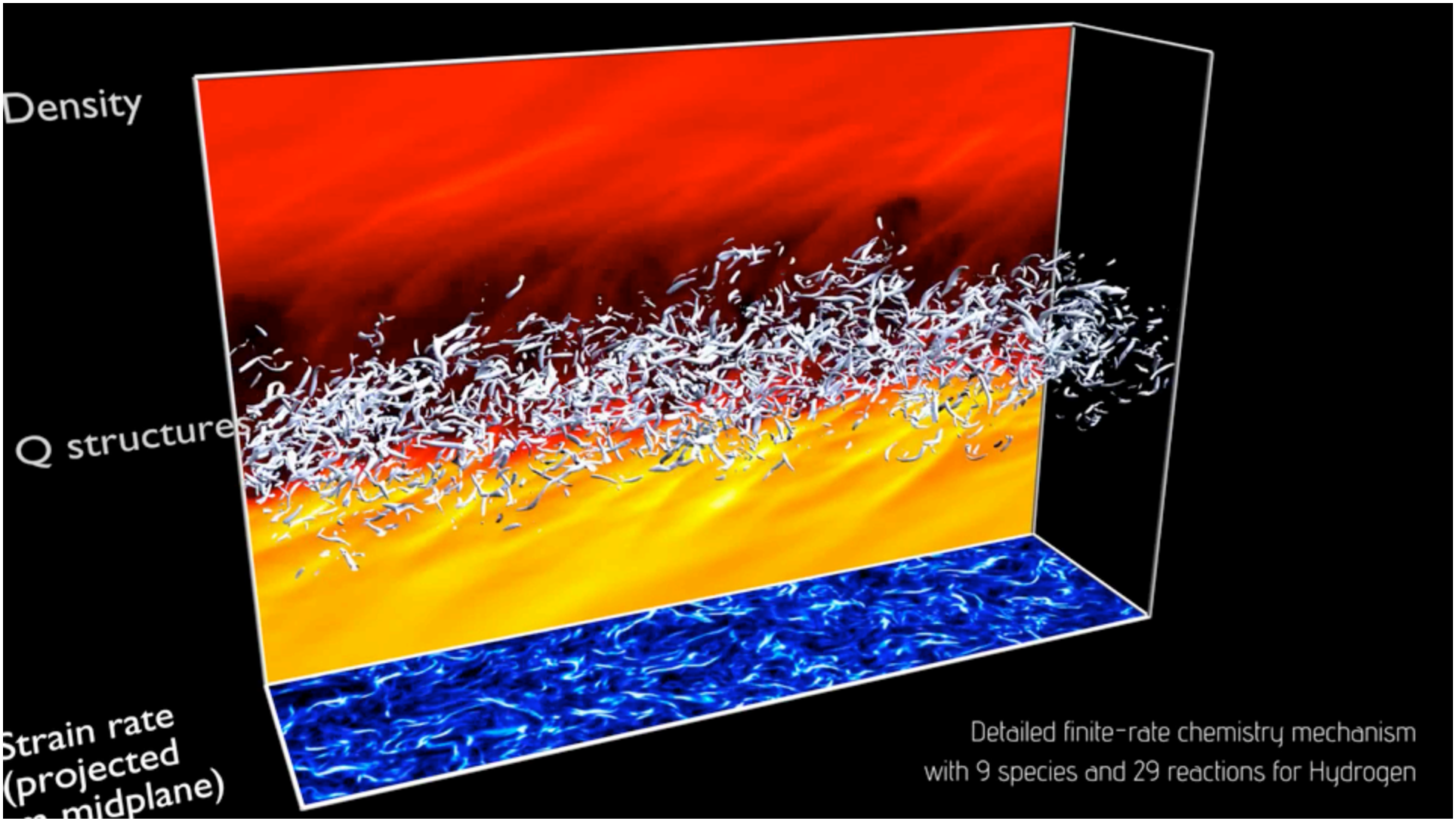


**Figure 4.8:** DNS of a premixed flame interacting with three-dimensional isotropic turbulence (Boger et al.[47]). An isosurface of temperature is visualized. The reaction rate is presented in two planes which are normal to the mean flame front. The vorticity field, corresponding to turbulent motions, is also displayed in the bottom plane.

# DNS




A. Saghafian

# RANS vs LES

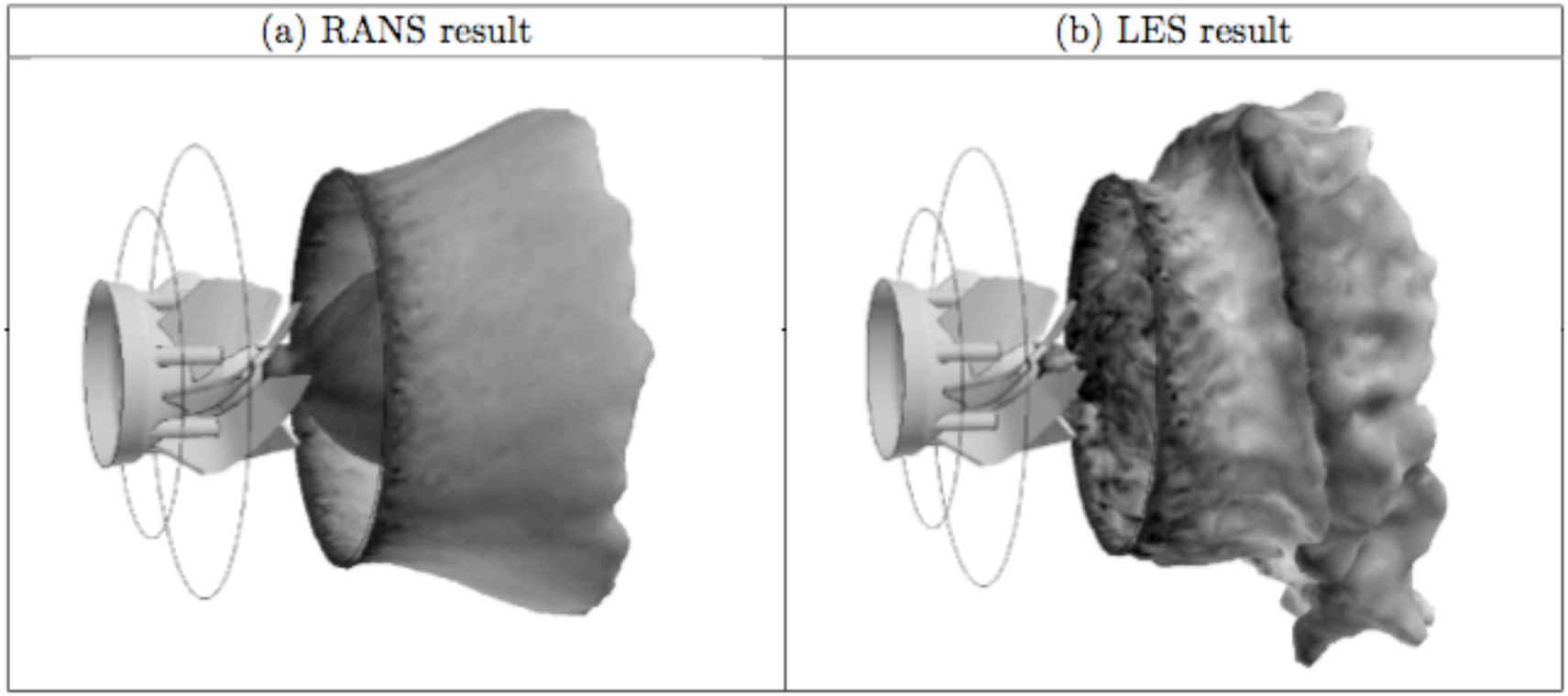



**Figure 4.9:** Isosurface of temperature (1100 K) during turbulent combustion in a swirled combustor (see geometry in § 10.3, Selle[474]). (a): RANS (mean field), (b): LES (instantaneous field).

# RANS vs LES

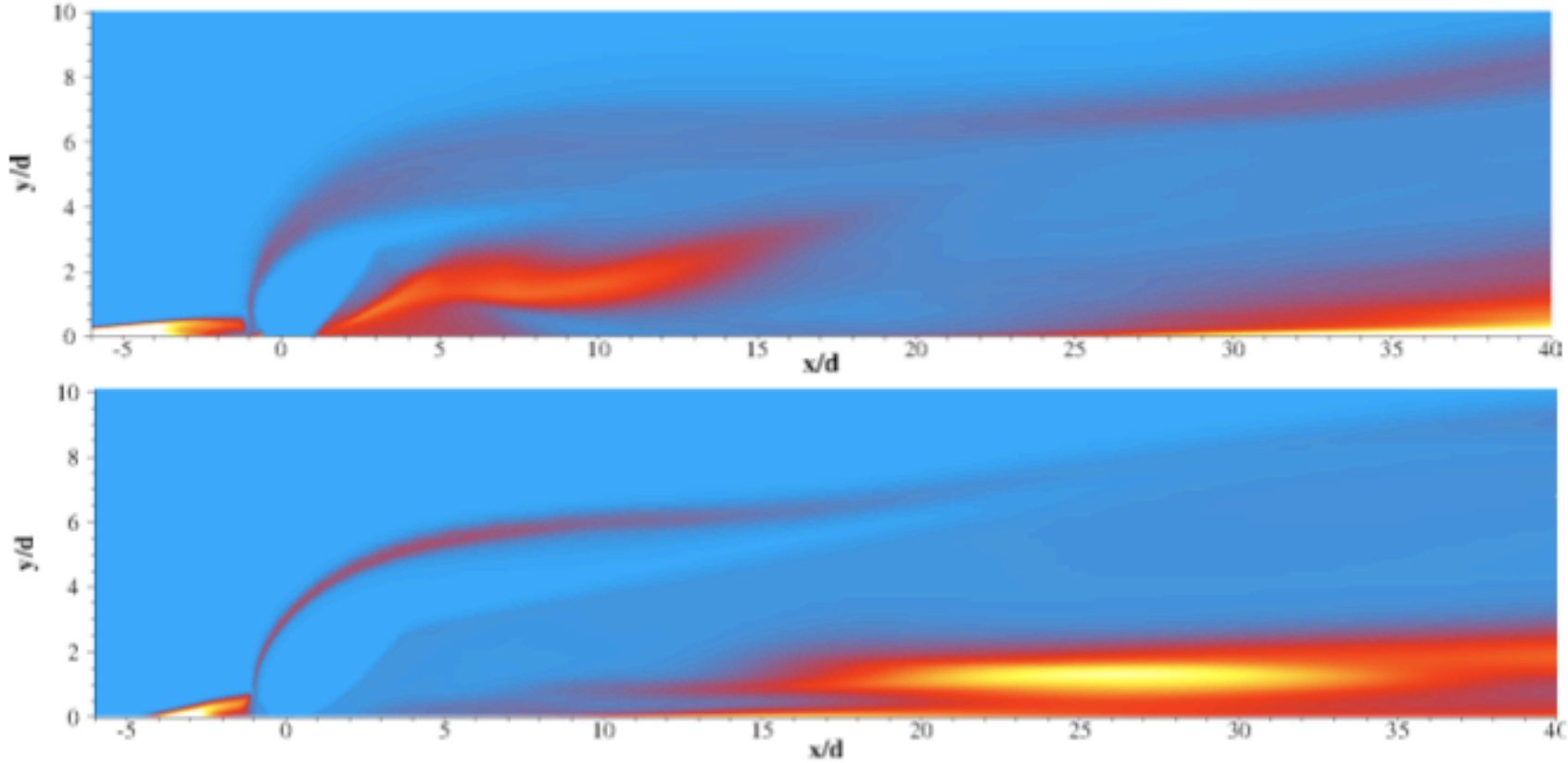
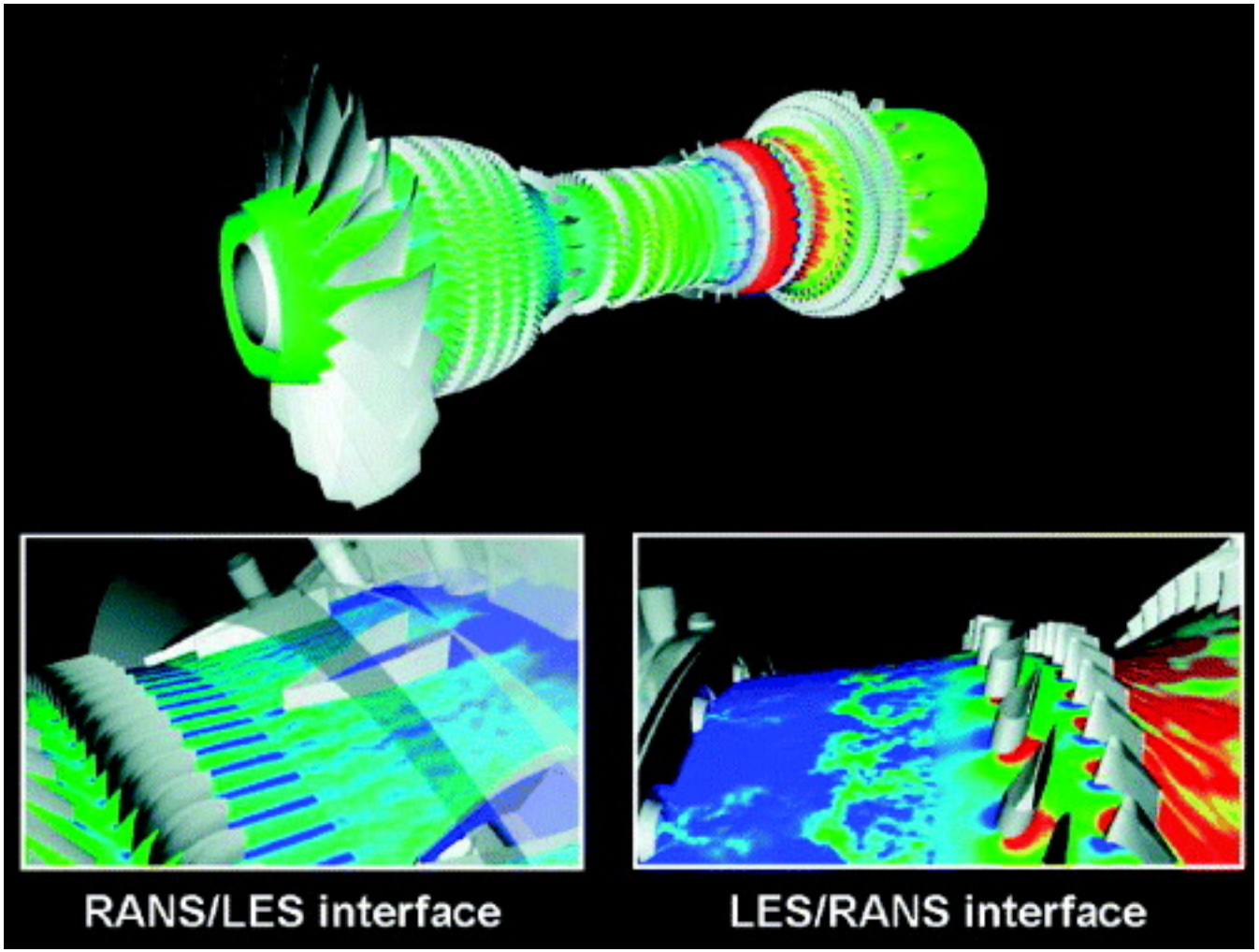



Figure 2.3: Time averaged OH mass fraction in the symmetry plane $z = 0$; LES (top) and RANS (bottom). Contours are from $\widetilde{Y}_{OH} = 0$ (blue), to $\widetilde{Y}_{OH} = 0.24$ (white).

Pecknik, Terrapon, Shagafian, Larsson

# RANS vs LES



# LES

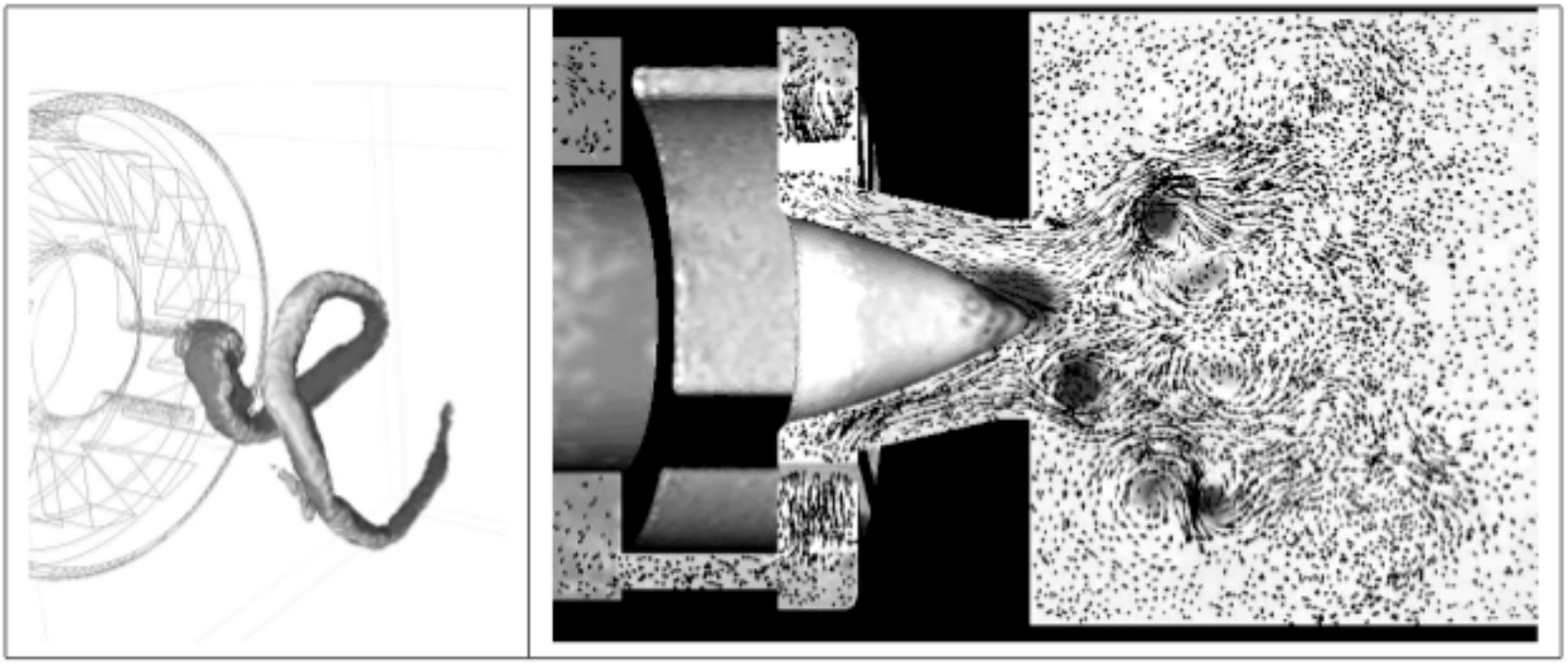
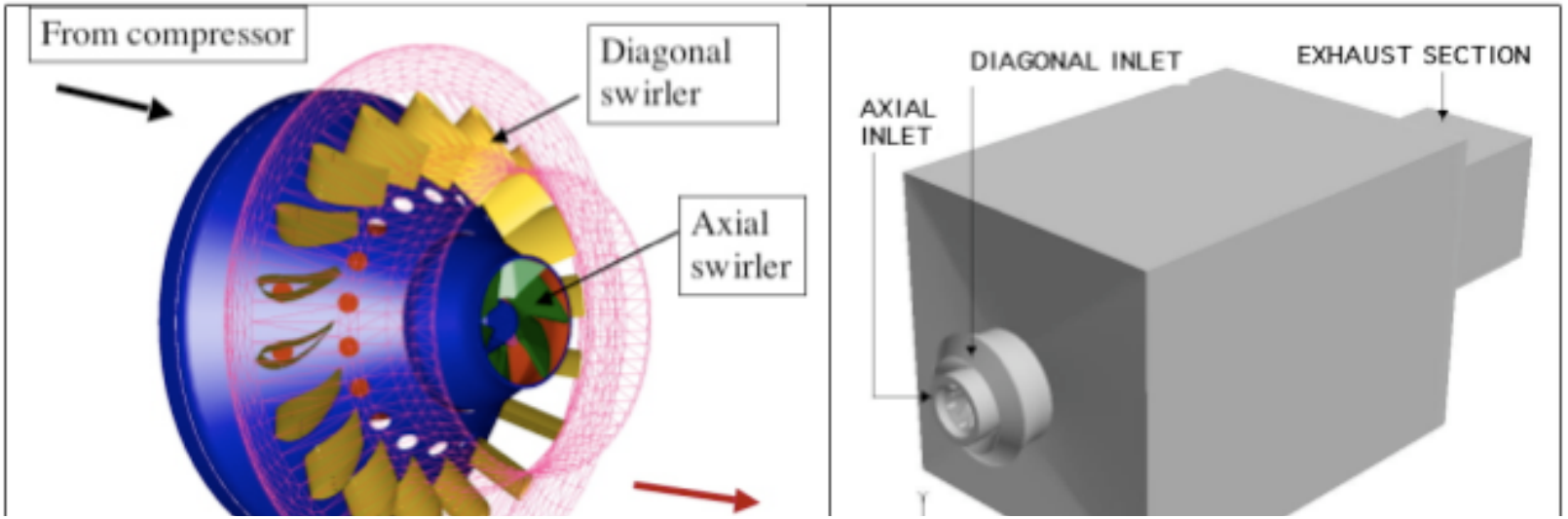


**Figure 10.6:** Visualization of the PVC mode in Case 1 using an isosurface of low pressure (left) and a field of pressure (gray scale) and velocity vectors in the central plane (right) (Lartigue[289]).

# LES



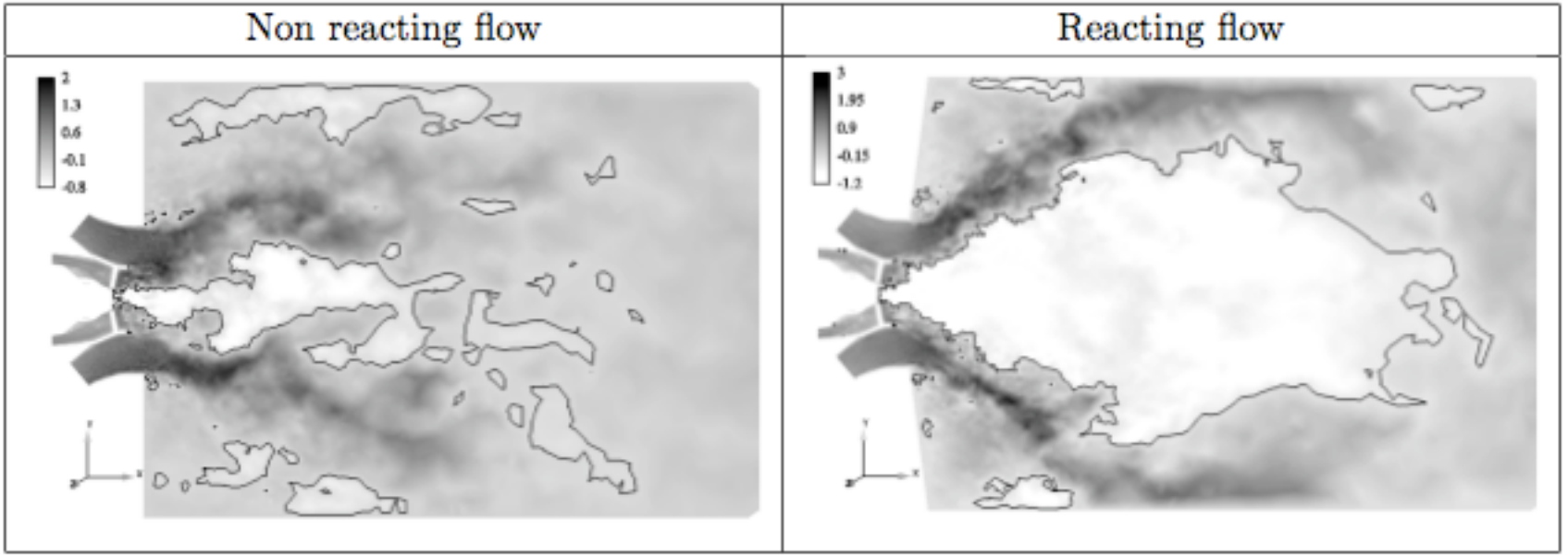
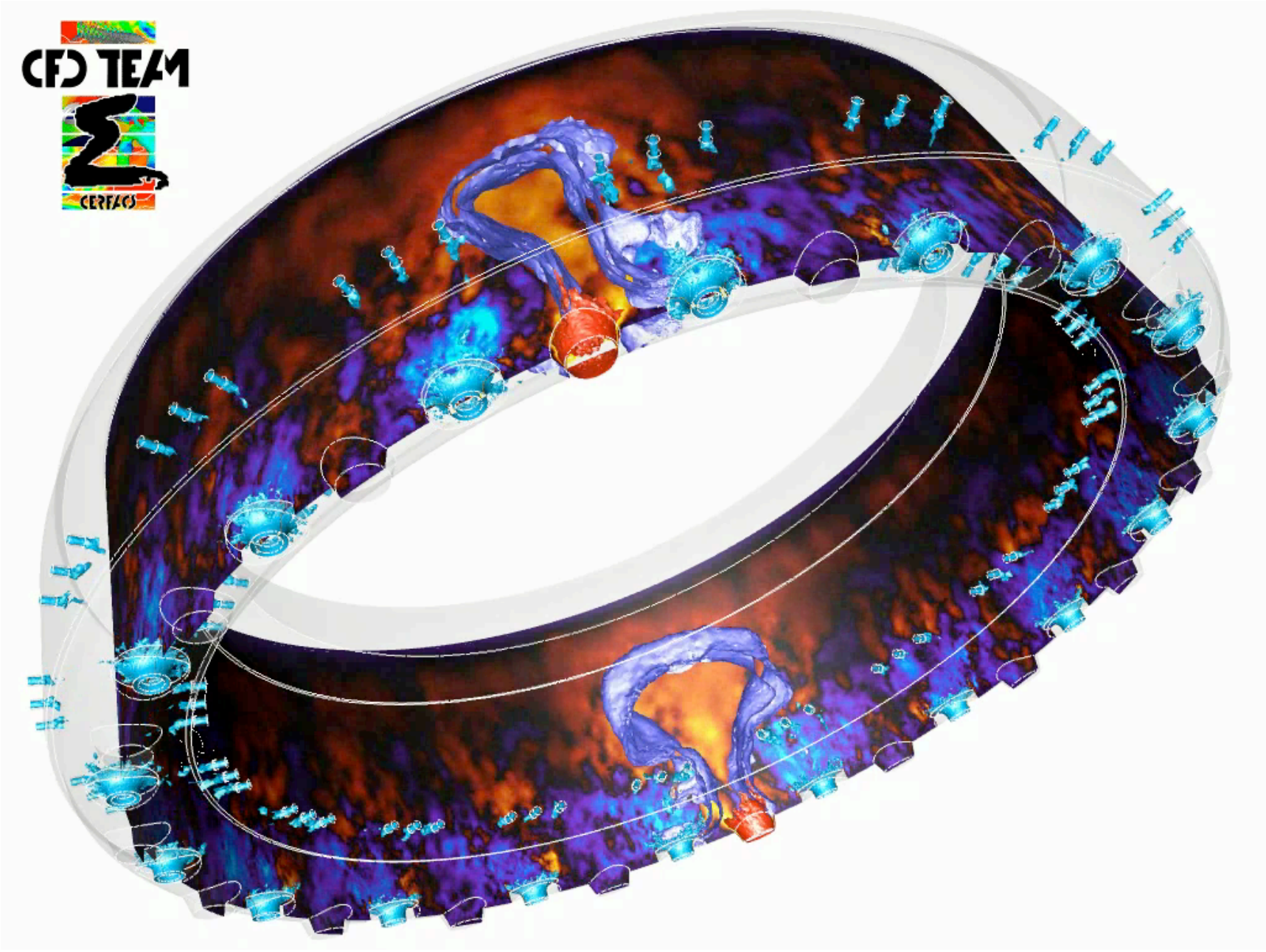
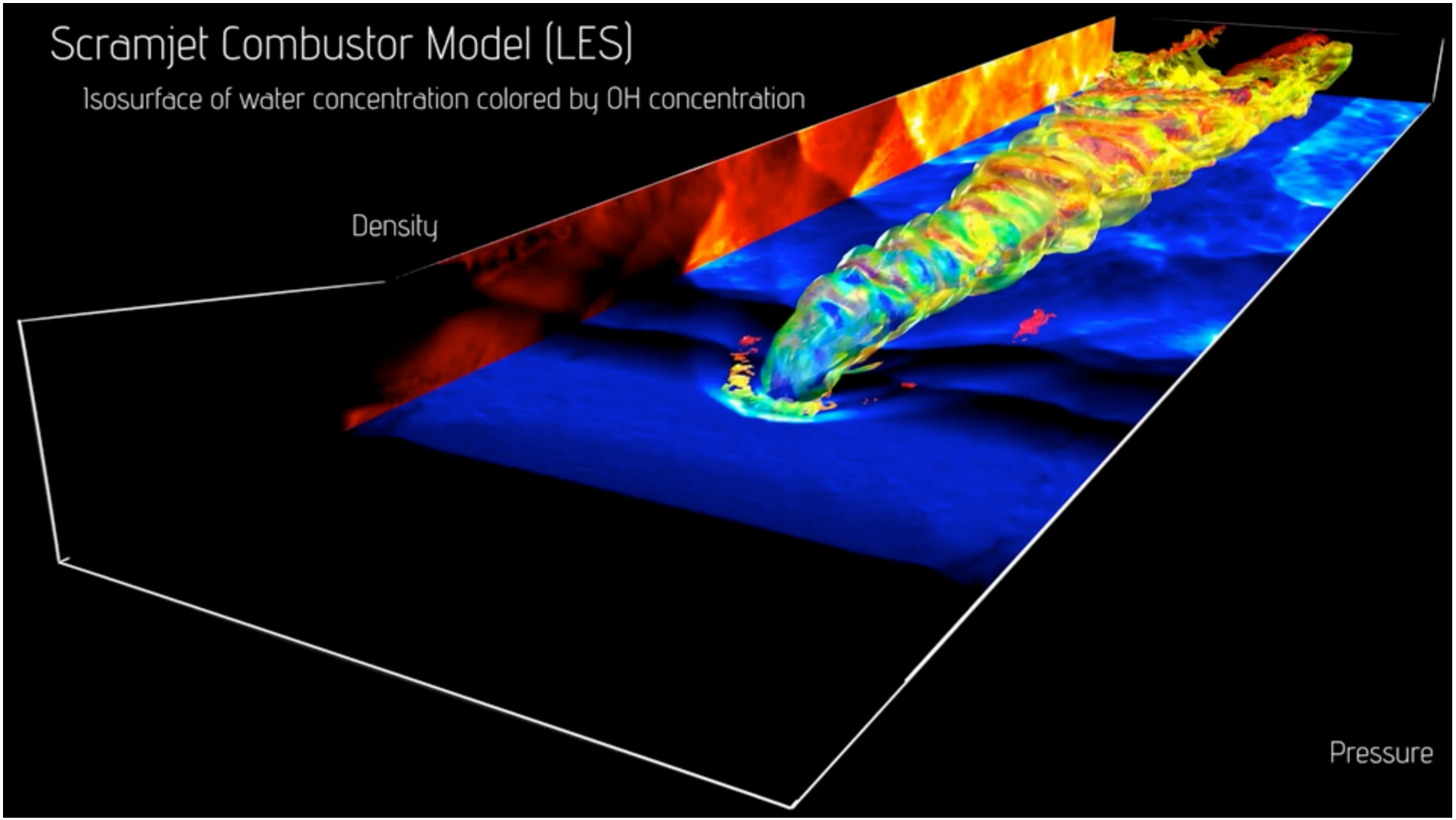




**Figure 10.15:** Comparison of cold (left) and reacting (right) instantaneous flow for Case 2 (axial velocity field displayed in central plane of the combustor). Black lines limit backflow regions (Selle[474]).

# LES



# LES




J. Larsson

STANFORD MECHANICAL ENGINEERING

**ME 471: TURBULENT COMBUSTION**

**Spring 2012**

# PART II:

# Turbulent Premixed Combustion

J. Urzay

PREMIXED TURBULENT COMBUSTION

## 1. REGIME DIAGRAMS IN PREMIXED TURBULENT COMBUSTION (PETERS VERSION)

ASSUME $Le_i = 1$ AND $Sc_\alpha = 1$ FOR SIMPLICITY, AND USE THE PREHEAT THICKNESS $\ell_F = \delta_L = \frac{D}{S_L}$, WITH $t_F = t_c = \frac{D}{S_L^2}$ THE FLAME TRANSIT TIME. THE FOLLOWING PARAMETERS ARE DEFINED:

- TURBULENT REYNOLDS NUMBER: $Re_\ell = \frac{u'\ell}{D} = \frac{u'\ell}{\ell_F S_L} = \left(\frac{\ell}{\ell_F}\right)\left(\frac{u'}{S_L}\right)$
- TURBULENT DAMKÖHLER NUMBER: $Da = \frac{T}{t_F} = \frac{\ell}{u'} \cdot \frac{S_L}{\ell_F} = \left(\frac{\ell}{\ell_F}\right)\left(\frac{S_L}{u'}\right)$
- TURBULENT KARLOVITZ NUMBER: $Ka = \frac{t_F}{\tau_K} = \frac{\ell_F^2}{\ell_K^2} = \frac{\nu^2}{S_L^2}$,

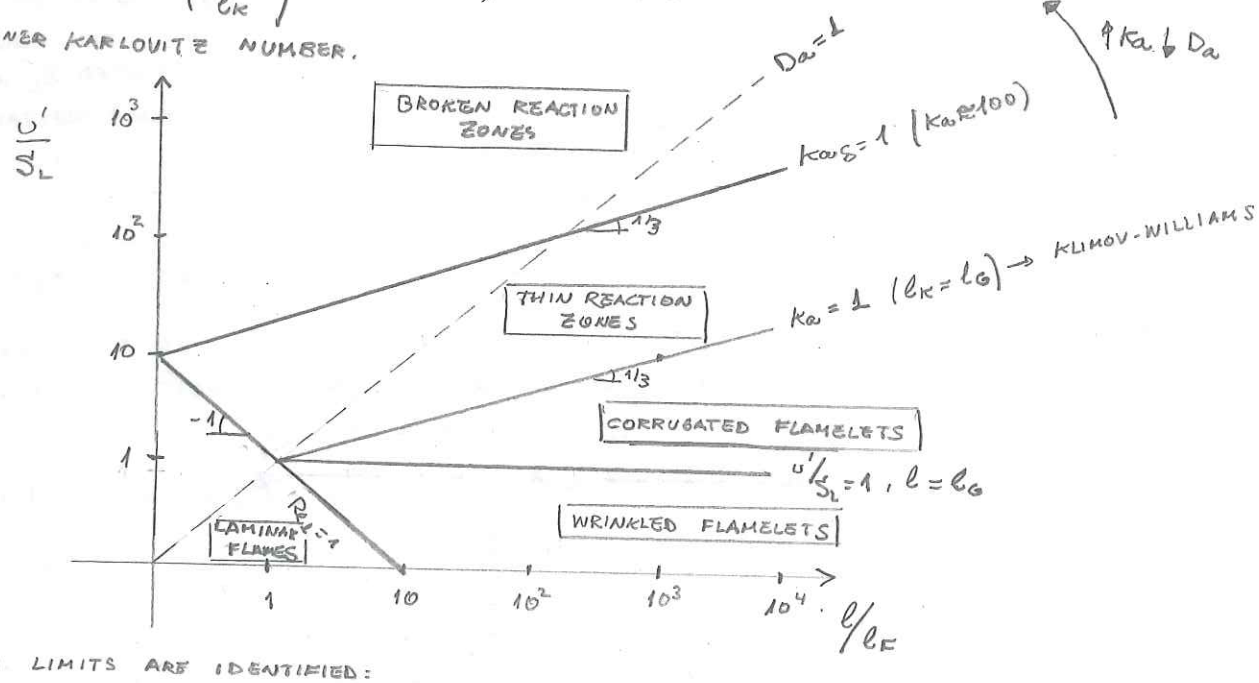
IN TERMS OF THE INTEGRAL MAGNITUDES $\ell$, $u'$ AND $T$, AND THE KOLMOGOROV SCALES $\ell_K$, $\nu$ AND $\tau_K$. USING THE DEFINITIONS ABOVE, THE RELATIONS

$$Re_\ell = Da^2 Ka^2 \quad \text{AND} \quad \frac{u'}{S_L} = Re_\ell\left(\frac{\ell_F}{\ell}\right) = Da^{-1}\left(\frac{\ell}{\ell_F}\right) = Ka^{2/3}\left(\frac{\ell}{\ell_F}\right)^{1/3}$$

ARE OBTAINED. FURTHERMORE, THERE EXISTS AN "INNER" KARLOVITZ NUMBER, BASED ON THE INNER REACTION-LAYER THICKNESS $\ell_\delta$, WHICH FOR HYDROCARBON COMBUSTION REPRESENTS THE FUEL-CONSUMPTION LAYER WHERE THE HYDROCARBON MOLECULES ARE ATTACKED BY THE RADICALS. IN PARTICULAR, $\ell_\delta \sim 0.1\,\ell_F$ IS TYPICALLY OBSERVED. THUS,

$$Ka_\delta = \left(\frac{\ell_\delta}{\ell_K}\right)^2 = \delta^2 Ka, \quad \text{WITH} \quad \delta \sim 0.1$$

IS THE INNER KARLOVITZ NUMBER.




THE FOLLOWING LIMITS ARE IDENTIFIED:

- $Re_\ell = 1$ DEFINES $\frac{u'}{S_L} = \frac{\ell_F}{\ell}$ AND $\frac{\ell^2}{D} = \frac{\ell}{u'}$ ⇒ NO SCALE DISPARITY.
- $Ka = 1$ DEFINES $\ell_F = \ell_K$ AND $t_F = \tau_K$ ⇒ FLAMES AS THICK AS THE KOLMOGOROV LENGTH AND AS SLOW AS THE KOLMOGOROV TIME.
- $Ka_\delta = 1$ DEFINES $\ell_\delta = \ell_F$ ⇒ INNER THICKNESS OF THE FLAME IS AS THICK AS THE KOLMOGOROV LENGTH.
- $Da = 1$ DEFINES $T = t_F$ ⇒ FLAMES AS SLOW AS THE INTEGRAL TIME SCALE.

REGIMES ($Re_\ell > 1$)

1. WRINKLED-FLAMELET REGIME: CHARACTERIZED BY $\frac{u'}{S_L} < 1$, $\frac{\ell_F}{\ell_K} < 1$, $\frac{\tau_F}{\tau_K} < 1$, $\frac{\nu}{S_L} < 1$, $\frac{T}{t_F} > 1$

$$\Rightarrow \boxed{Da > 1,\ Ka < 1,\ u'/S_L < 1}$$

IN THIS REGIME, THE TURNOVER TIME OF BOTH INTEGRAL AND KOLMOGOROV EDDIES IS MUCH LONGER THAN THE FLAME TRANSIT TIME. ADDITIONALLY, THE VELOCITY FLUCTUATIONS ARE SMALL AND EDDIES CANNOT CONVOLUTE THE FLAME FRONT ENOUGH TO FORM MULTIPLY-CONNECTED SURFACES.

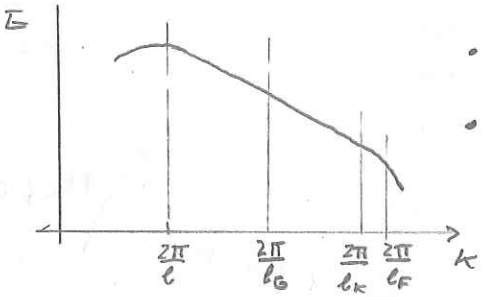
ORDERING OF SCALES: $\ell_F < \ell_K < \ell$, $t_F < \tau_K < T$, $\nu < u' < S_L$

2. CORRUGATED-FLAMELET REGIME: CHARACTERIZED BY $\boxed{\frac{u'}{S_L} > 1,\ Da > 1,\ Ka < 1}$

LARGE EDDIES CAN PUSH THE FLAME AROUND AND FORM CONVOLUTED REGIONS, BUT THE SMALLEST EDDIES WILL NOT PENETRATE IN THE FLAME AND WILL NOT WRINKLE THE FLAME FRONT.

ORDERING OF SCALES: $\ell_F < \ell_K < \ell$, $t_F < \tau_K < T$, $\nu < S_L < u'$

IN THIS REGIME, THERE IS A CHARACTERISTIC LENGTH, THE GIBSON SCALE $\ell_G = \frac{S_L^3}{\varepsilon}$, ABOVE WHICH EDDIES INTERACT WITH THE FLAME AND CORRUGATE IT. SINCE $\frac{\ell_G}{\ell} = \frac{S_L^3}{u'^3} < 1$ IN THIS REGIME, THEN




- FOR $\ell_m < \ell_G$, THEN $U_m < S_L \Rightarrow$ EDDIES OF SIZE $\ell_m$ CANNOT WRINKLE THE FLAME
- FOR $\ell_m > \ell_G$, THEN $U_m > S_L \Rightarrow$ EDDIES OF SIZE $\ell_m$ HAVE TURNOVER VELOCITIES $V_m$ THAT EXCEED $S_L$ AND THEREFORE CAN CAUSE SUBSTANTIAL CORRUGATION.
- FOR $u' = S_L \Rightarrow \ell = \ell_G$
- FOR $\nu = S_L \Rightarrow \ell_G = \ell_K$

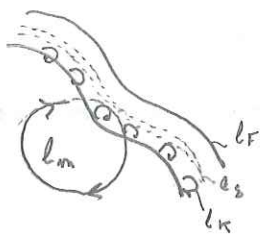
3. THIN REACTIONS REGIME: CHARACTERIZED BY $\boxed{\frac{u'}{S_L} > 1,\ Ka > 1,\ Da \gtrsim 1,\ Ka_\delta < 1}$

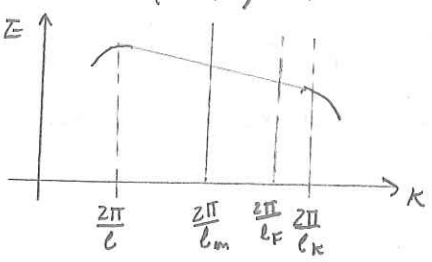
IN THIS REGIME, THE SMALLEST EDDIES CAN ENTER INTO THE CONVECTIVE-DIFFUSIVE ZONE OF THE FLAME, BUT THEY ARE STILL LARGER THAN THE INNER-LAYER THICKNESS $\ell_\delta$. THUS, THE KOLMOGOROV EDDIES CAN PUSH THE FLAME AROUND IT AND EVEN EXTINGUISH IT:

ORDERING OF SCALES: $\ell_\delta < \ell_K < \ell_F < \ell$, $t_\delta < \tau_K < t_F < T$ $(Da > 1)$ OR

$t_\delta < \tau_K < T < t_F$ $(Da < 1)$, $S_L < \nu < u'$

IN THIS REGIME, THERE EXISTS AN EDDY SIZE $\ell_m$ SUCH THAT ITS TURNOVER TIME EQUALS THE FLAME TRANSIT TIME: $\ell_m = (\varepsilon t_F^3)^{1/2}$, SO THAT $\frac{\ell_m}{\ell_F} = \frac{v_m}{S_L} > 1$, , $\ell_m$ = ZIMONT SCALE ZIMONT (1979)




DURING ITS TURNOVER TIME, AN EDDY OF SIZE $\ell_m$ WILL INTERACT WITH THE ADVANCING REACTION FRONT AND WILL BE ABLE TO TRANSPORT PREHEATED MIXTURE OVER DISTANCES OF ORDER $\ell_m$. $\ell_m$ IS THE MAXIMUM DISTANCE THAT A PARCEL OF PREHEATED MIXTURE CAN BE TRANSPORTED AHEAD OF THE FLAME

$\Rightarrow$ CAUSES FLAME BROADENING.

4. BROKEN REACTIONS: CHARACTERIZED BY: $\boxed{\frac{u'}{S_L} > 1,\ Ka_\delta > 1,\ Da \lesssim 1}$

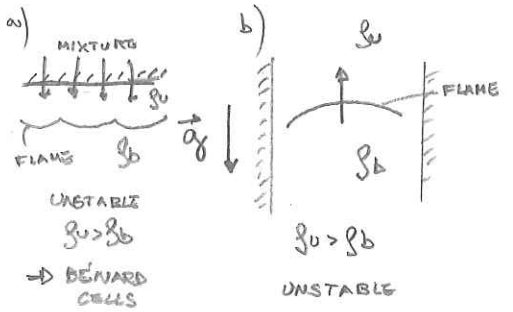
IN THIS REGIME, THE KOLMOGOROV EDDIES CAN ENTER IN THE REACTION REGION AND CAUSE EXTINCTION.

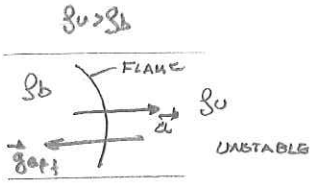
ORDERING OF SCALES: $\ell_K < \ell_\delta < \ell_F < \ell$, $\tau_K < t_\delta < T < t_F$ $(Da < 1)$, $S_L < \nu < u'$

$\tau_K < t_\delta < t_F < T$ $(Da > 1)$

## 2. PREMIXED-FLAME INTRINSIC INSTABILITIES

- **BODY-FORCE INSTABILITIES:** MAINLY CAUSED BY GRAVITY AND GENERATED BY THE RAYLEIGH-TAYLOR MECHANISM, BY WHICH A LESS-DENSE FLUID BENEATH A MORE DENSE FLUID IS BUOYANTLY (OR INERTIALLY) UNSTABLE. (REMINDER: $\rho_u / \rho_b$ BY THERMAL EXPANSION)



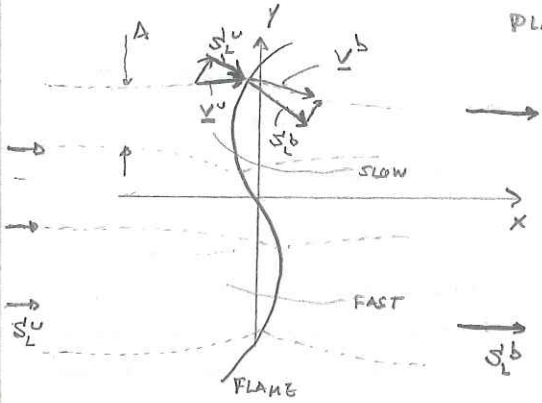




AN ACCELERATING FLAME IS SUBJECT TO AN EFFECTIVE GRAVITY $\vec{g}_{eff}$

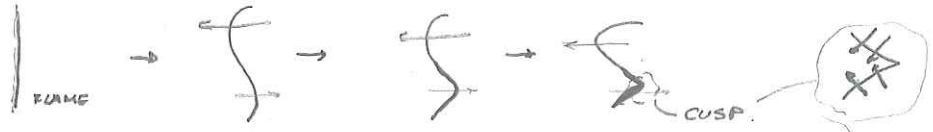
⇒ THESE INSTABILITIES HAVE A LONG WAVELENGTH (OF ORDER $S_L^2/g \sim (Dm)^{-2}$) AND LONG GROWTH TIMES (OF ORDER $S_L/g \sim 10^{-2}\,s$)

FOR DECELERATING FLAMES, FLAMES PROPAGATING DOWNWARD OR BURNER-STABILIZED FLAMES WITH THE FLOW UPWARD, THE BODY-FORCE EFFECTS ARE STABILIZING. BUOYANCY EFFECTS ARE FAR FIELD PHENOMENA THAT STABILIZE OR INSTABILIZE DEFLAGRATIONS WITHOUT APPRECIABLY MODIFYING THE FLAME STRUCTURE (NOTICE THAT THIS MAY NOT HOLD FOR OTHER TYPES OF BODY FORCES LIKE ELECTRIC FIELDS, WHICH MAY DISRUPT THE INNER REACTIVE-DIFFUSIVE REGION BY PUSHING IONS AROUND).

- **HYDRODYNAMIC INSTABILITIES:** INDEPENDENTLY DISCOVERED BY DARRIEUS AND LANDAU, IT IS USUALLY TERMED THE "DARRIEUS-LANDAU" INSTABILITY, WHICH STATES THAT THE PLANAR DEFLAGRATION IS UNCONDITIONALLY UNSTABLE BECAUSE OF THERMAL EXPANSION



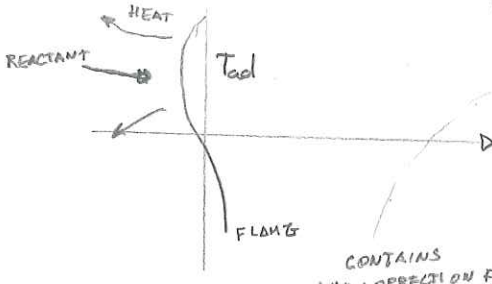

IF THE PLANAR FLAME IS PERTURBED, THEN CONTINUITY OF THE COMPONENT OF VELOCITY TANGENTIAL TO THE FLAME IMPLIES THAT THE STREAMLINES MUST DIVERGE AHEAD OF A BULGE PROTUDING INTO THE FRESH MIXTURE AND CONVERGE BEHIND THIS BULGE. SINCE MASS CONSERVATION NEEDS TO BE SATISFIED, IT IS SEEN THAT THE STREAMWISE VELOCITY COMPONENT OF $\underline{v}^u$ IS SMALLER THAN $S_L^u$ JUST AHEAD OF THE BULGE, THEREFORE LOCALLY THE BULGE PROPAGATES FASTER THAN THE LOCAL FLOW VELOCITY. THE CONTRARY HAPPENS IN THE FLAME VALLEYS.




THE D-L INSTABILITY IS OF A PURELY DIVERGING, NON-OSCILLATORY CHARACTER, WITH AN EXPONENTIAL GROWTH $e^{+\sigma t}$ WHERE $\sigma = \frac{k}{1+\rho_b/\rho_u}\left\{\left[1+\frac{\rho_b^2/\rho_u^2-1}{\rho_b/\rho_u}\right]^{1/2}-1\right\}$, WHICH TENDS TO $\frac{\rho_u-\rho_b}{\rho_b}$ FOR SMALL → ALL WAVELENGTHS! EXPANSION RATIOS.

DIFFUSIVE-THERMAL PHENOMENA AND BUOYANCY EFFECTS INTRODUCE STABILIZING EFFECTS. IN PARTICULAR, BUOYANCY STABILIZES DEFLAGRATIONS FOR WAVELENGTHS LARGER THAN $S_L^2/g$. LAMINAR DEFLAGRATIONS ARE OBSERVED EXPERIMENTALLY BECAUSE OF THESE STABILIZATION EFFECTS.

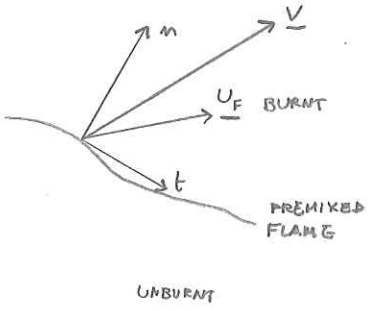
- **DIFFUSIVE-THERMAL INSTABILITIES:** STABILIZE D-L INSTABILITIES AT SHORT WAVELENGTHS (OF $O(\delta_L)$) AND ENABLE STEADY, PLANAR FLAMES TO BE SEEN IN THE LABORATORY IF Le IS NOT TOO SMALL. FOR $Le \lesssim 0.5$ HEAT IS LOST FROM THE BULGE SLOWER THAN IT CAN BE GENERATED BY THE DIFFUSION OF THE REACTANT INTO THE REACTION ZONE ⇒ $T_{ad}$ IS INCREASED AT THE FORWARD POINTING BULGE AND THE FLAME MOVES FASTER IN THIS REGION ⇒ UNSTABLE. ⇒ ENHANCES HYDRODYNAMIC INSTABILITIES




CONTAINS THE CORRECTION FOR FINITE THICKNESS AND THERMAL EXPANSION!

EX: CELLULAR INSTABILITIES IN LEAN HYDROGEN FLAMES!

## KINEMATIC BALANCE




THE KINEMATIC BALANCE IN THE NORMAL DIRECTION TO THE FLAME FRONT REQUIRES:

$$S_{u,b} = \left( \underline{v}_{u,b} - \underline{U}_F \right) \cdot \underline{n}$$

WHERE THE SUBINDEXES $u,b$ DENOTE UNBURNT OR BURNT CONDITIONS, RESPECTIVELY, $\underline{v}$ IS THE LOCAL FLOW VELOCITY AND $\underline{U}_F$ IS THE VELOCITY OF THE FRONT IN THE LABORATORY FRAME. NOTE THAT $\underline{v}_u \neq \underline{v}_b$ BECAUSE OF THERMAL EXPANSION, AND

$$\rho_u \left( \underline{v}_u - \underline{U}_F \right) \cdot \underline{n} = \rho_b \left( \underline{v}_b - \underline{U}_F \right) \cdot \underline{n}$$

BY CONTINUITY ACROSS THE FLAME. ADDITIONALLY, THE TANGENTIAL COMPONENT OF THE VELOCITY IS CONTINUOUS SINCE THE PRESSURE VARIATIONS ARE NEGLIGIBLE: $\underline{v} \cdot \underline{t} = \underline{U}_F \cdot \underline{t}$

## PREMIXED TURBULENT-COMBUSTION MODELLING

CLASSIC MODELS OF TURBULENT COMBUSTION IN RANS ARE BASED ON THE PROGRESS VARIABLE EQUATION AS FOLLOWS. CONSIDER A 1-STEP CHEMISTRY, WITH REACTION RATE $\dot{w}_F = B \rho Y_F e^{-T_a/T}$, AND ASSUME UNITY LEWIS NUMBER, SMALL MACH NUMBER AND CONSTANT $c_p$. THEN

$$\left.\begin{aligned} \rho \underline{v} \cdot \nabla Y_F &= \nabla \cdot (\rho D \nabla Y_F) - \dot{w}_F \\ \rho c_p \underline{v} \cdot \nabla T &= \nabla \cdot (\kappa \nabla T) - \dot{w}_T \end{aligned}\right\}$$

DEFINING $Y = Y_F / Y_{Fu}$ AND $c = \dfrac{c_p (T - T_u)}{Q Y_{Fu}} = \dfrac{T - T_u}{T_b - T_u}$, (SEE PAGE 7 FOR NOTATION)

THEN $c + Y = 1$ ($\leftarrow$ Le=1). IN PARTICULAR, $c$ IS A PROGRESS VARIABLE, WITH $c = 1$ IN THE BURNT SIDE AND $c = 0$ IN THE UNBURNT SIDE.

AFTER THE FAVRE DECOMPOSITION IS PERFORMED, THE PROBLEM OF THE TURBULENT PREMIXED FLAME BECOMES

$$\left.\begin{aligned} &\nabla \cdot \left( \bar{\rho} \tilde{\underline{u}} \right) = 0 \\ &\bar{\rho} \frac{\partial \tilde{u}}{\partial t} + \bar{\rho} \tilde{\underline{u}} \cdot \nabla \tilde{u} = -\nabla \bar{P} - \nabla \cdot \left( \bar{\rho} \widetilde{\underline{u}'' u''} \right) + \nabla \cdot \bar{\tau}' \\ &\bar{\rho} \frac{\partial \tilde{c}}{\partial t} + \bar{\rho} \tilde{\underline{u}} \nabla \tilde{c} = -\nabla \cdot \left( \bar{\rho} \widetilde{\underline{c}'' \underline{c}''} \right) + \nabla \cdot \left( \overline{\rho D \nabla c} \right) + \bar{\dot{w}}_c \end{aligned}\right\}$$

CLOSURE IS NEEDED FOR THE TURBULENT FLUXES AND THE MEAN REACTION RATE. THE TURBULENT FLUXES CAN BE CLOSED WITH $k$-$\varepsilon$ TYPE OF MODELS. (SEE PAGE 12)

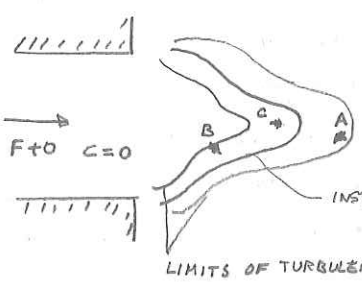
## EDDY BREAK-UP MODEL (SPALDING, 1971)

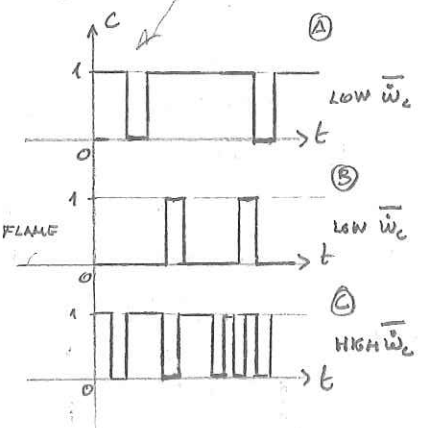
THE CASCADE PROCESS OF MIXING CONTROLS THE CHEMICAL REACTIONS AS LONG AS MIXING RATHER THAN CHEMISTRY IS THE RATE-DETERMINING PROCESS. IN THE EBU MODEL, THE MEAN REACTION RATE IS MODELLED AS

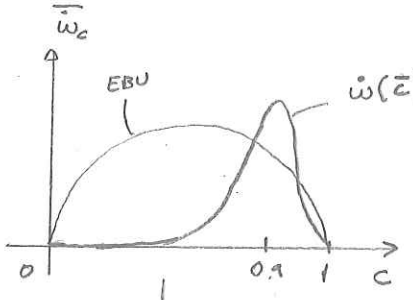
$$\bar{\dot{w}}_c = \bar{\rho} C_{EBU} \frac{\left( \widetilde{c''^2} \right)^{1/2}}{\tau}, \quad \text{WITH } \tau = k/\varepsilon \text{ THE INTEGRAL TIME SCALE AND } C_{EBU} \text{ AN ADJUSTABLE CONSTANT.}$$

IN THIS FORMULATION, $\widetilde{c''^2}$ CAN BE OBTAINED BY SOLVING A TRANSPORT EQUATION FOR THE VARIANCE (WHICH WOULD NEED MODELLING), OR BY USING A RANDOM TELEGRAPHIC SIGNAL FOR VANISHING THICKNESS OF THE REACTION LAYER:

$$\bar{\rho} \widetilde{c''^2} = \overline{\rho c''^2} = \overline{\rho (c - \tilde{c})^2} = \bar{\rho} \left( \tilde{c}^2 - \tilde{c}^2 \right) \approx \bar{\rho} \tilde{c} (1 - \tilde{c}) \quad \left( \hookrightarrow c^2 \sim c \right)$$



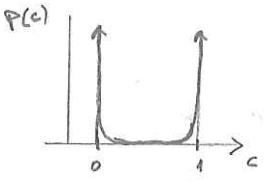




EBU MODEL PREDICTS A BROADER REACTION RATE THAN THE APPROX $\dot{w}(\tilde{c})$

ALTHOUGH ATTRACTIVE AND SIMPLE, THE EBU MODEL DOES NOT INCLUDE ANY CHEMICAL-KINETIC EFFECTS, AND IT TENDS TO FAIL IN HIGHLY STRAINED REGIONS WHERE $\frac{1}{\tau} = \frac{\varepsilon}{k}$ IS LARGE, LIKE IN FLAME HOLDERS AND NEAR WALLS.

## BRAY-MOSS-LIBBY MODEL (1977)

THIS MODEL ASSUMES A PDF FOR $c$ THAT HAS TWO PEAKS AND IS GIVEN BY TWO DELTA FUNCTIONS:




$$P(c;\underline{x},t) = \underbrace{A(\underline{x},t)\,\delta(c)}_{①} + \underbrace{B(\underline{x},t)\,\delta(1-c)}_{②} + \underbrace{C(\underline{x},t)\,f(c)}_{③}$$

IN THE INFINITESIMALLY-THIN REACTION-LAYER APPROXIMATION, $C \to 0$ AND INTERMEDIATE STATES BETWEEN BURNT/UNBURNT ARE HIGHLY UNLIKELY.

① : PROBABILITY OF FINDING UNBURNT GAS
② : " " BURNT "
③ : " " " REACTING GAS.

NORMALIZATION: $\int_0^1 P(c)\,dc = A + B = 1$

BASED ON THIS PDF, AND FOR ANY FUNCTION $f \Rightarrow \overline{f} = \int_0^1 f(c)\,P(c)\,dc = A\overline{f}_u + B\overline{f}_b$

THEN $\boxed{\overline{c} = B}$, SINCE $\overline{c}_u = 0$ AND $\overline{c}_b = 1$, AND $\tilde{c} = \frac{\overline{\rho c}}{\overline{\rho}} = \frac{\rho_b B}{\overline{\rho}}$ WITH $\overline{\rho} = A\rho_u + B\rho_b$.

ALSO, IF THE AVERAGE MOLECULAR WEIGHT IS ASSUMED TO BE CONSTANT, $\overline{W}_b = \overline{W}_u$, THEN $\frac{\overline{\rho}}{\rho_u} = \frac{T_u}{\overline{T}}$

$$\Rightarrow \overline{\rho T} = \overline{\rho}\,\tilde{T} = \overline{\rho}\left[(T_b - T_u)\,\tilde{c} + T_u\right] = \rho_u T_u \Rightarrow \begin{cases} \frac{\overline{\rho}}{\rho_u} = \frac{1-\alpha}{1-\alpha(1-\tilde{c})}, \text{ WITH } \alpha = \frac{\rho_u - \rho_b}{\rho_u} \\ \tilde{T} = T_u\left(\frac{\rho_u}{\overline{\rho}}\right) = T_u\left[\frac{1-\alpha(1-\tilde{c})}{1-\alpha}\right] \end{cases} \Rightarrow B = \frac{\tilde{c}}{1-\alpha(1-\tilde{c})}$$

$$\Rightarrow A = \frac{(1-\tilde{c})(1-\alpha)}{1-\alpha(1-\tilde{c})}$$

A RELATION BETWEEN FAVRE AND REYNOLDS AVERAGES CAN BE OBTAINED WITHIN THE BML FRAMEWORK AS FOLLOWS: $\tilde{f} = A\frac{\rho_u}{\overline{\rho}}\overline{f}_u + B\frac{\rho_b}{\overline{\rho}}\overline{f}_b = (1-\tilde{c})\overline{f}_u + \tilde{c}\overline{f}_b$, AND IN PARTICULAR,

$$\boxed{\overline{c} = \frac{\tilde{c}}{1-\alpha(1-\tilde{c})} = B}$$

$\Rightarrow$ CLOSED RELATIONSHIP BETWEEN $\overline{c}$ AND $\tilde{c}$, WITH

$$\overline{\rho c''} = \overline{\rho}(\tilde{c} - \overline{c}) = \overline{\rho}\tilde{c}\left(1 - \frac{1}{1-\alpha(1-\tilde{c})}\right)$$

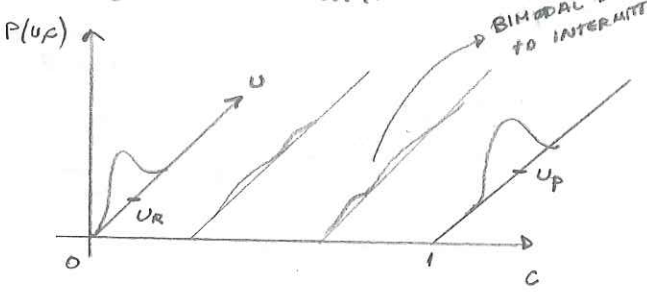
↳ RECALL THAT $\overline{\rho}\tilde{c} = \overline{\rho}\overline{c} + \overline{\rho c''}$

$\Rightarrow$ THE DIFFERENCE BETWEEN $\tilde{c}$ AND $\overline{c}$ INCREASES AS $\alpha$ INCREASES.

THE SCALAR VARIANCE CAN BE OBTAINED USING THE BML MODEL:

$$\overline{\rho c''c''} = \overline{\rho c''c''} = \int_0^1 \rho(c-\tilde{c})^2 P(c;\underline{x},t)\,dc = B\rho_b(1-\tilde{c}) = \overline{\rho}\tilde{c}(1-\tilde{c}).$$

THE TURBULENT FLUXES OF SCALAR CAN BE OBTAINED BY USING A JOINT PDF BETWEEN THE PROGRESS VARIABLE AND THE VELOCITY:




$$P(c,u;\underline{x},t) = A(\underline{x},t)\,\delta(c)\,P_u(0,u;\underline{x},t) + B(\underline{x},t)\,\delta(1-c)\,P_b(1,u;\underline{x},t) + C(\underline{x},t)\,f(c,u;\underline{x},t)$$

SUCH THAT $P_u$ IS THE CONDITIONAL PDF OF VELOCITY IN THE REACTANTS AND $P_b$ IS THE CONDITIONAL PDF OF VELOCITY IN THE PRODUCTS.

THEN $\overline{\rho u''c''} = \overline{\rho u''c''} = \int_0^\infty\int_0^1 \rho(c-\tilde{c})(u-\tilde{u})\,P(c,u;\underline{x},t)\,dc\,du = \overline{\rho}\tilde{c}(1-\tilde{c})(\overline{u}_b - \overline{u}_u)$ FOR $C \to 0$,

WHERE $\overline{u}_b$ AND $\overline{u}_u$ ARE THE VELOCITIES CONDITIONED ON THE PRODUCTS AND REACTANT SIDES, RESPECTIVELY.

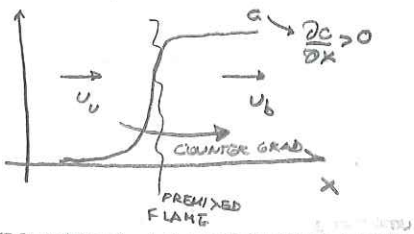
NOTICE THAT, SINCE $u_b > u_u$ BECAUSE OF THERMAL EXPANSION, THEN $\overline{\rho}\,\widetilde{u''c''} > 0 \Rightarrow$ COUNTERGRADIENT TRANSPORT

SOLUTION → USE TRANSPORT EQUATIONS FOR SECOND MOMENTS ($\widetilde{u''c''}$, $\widetilde{u''u''}$) (WHICH ARE UNCLOSED!)

## TURBULENT TRANSPORT IN PREMIXED FLAMES (LIBBY + BRAY, 1981)

THE BML MODEL REVEALS THAT TURBULENT TRANSPORT THROUGH A PREMIXED FLAME GOES IN THE OPPOSITE DIRECTION AS THAT PREDICTED BY GRADIENT FORMULATIONS OF THE TYPE:

$$\overline{\rho u'' c''} = -\frac{\mu_t}{Sc_t}\frac{\partial \tilde{c}}{\partial x}.$$




IN PREMIXED FLAMES, THE GRADIENT $\partial c/\partial x$ IS POSITIVE THROUGH THE FLAME. BECAUSE OF THERMAL EXPANSION, THE FLOW IS STRONGLY ACCELERATED ON THE BURNT SIDE, WHICH RESULTS IN A PREFERENTIAL TRANSPORT OF PRODUCTS DOWNSTREAM. THIS MECHANISM IS ABSENT FROM STANDARD GRADIENT-TRANSPORT MODELS, THEREBY REPRESENTING A "COUNTERGRADIENT" DIFFUSION. OTHER MODELLING APPROACHES, SUCH AS LEVEL SET, OR MIXTURE-FRACTION FORMULATIONS FOR NON-PREMIXED COMBUSTION, ARE EXEMPTED FROM THIS EFFECT.

COUNTERGRADIENT DIFFUSION } LOW TURBULENCE LEVELS, HIGH THERMAL EXPANSION

GRADIENT DIFFUSION } HIGH TURBULENCE LEVELS, LOW THERMAL EXPANSION

**REACTION RATE MODELLING:** (BRAY + LIBBY + MOSS, 1984)

A CENTRAL ASSUMPTION OF THE BML MODEL IS THAT THE FLAME-INTERIOR CONTRIBUTION TO THE PDF VANISHES AS $C \to 0$. THEREFORE, THE BML FORMULATION CANNOT BE USED FOR EVALUATING THE REACTION RATE:

$$\overline{\dot{\omega}_c} = \int_0^1 \dot{\omega}_c(c)\, P(c;x,t)\, dc = \mathcal{C}(x,t)\int_0^1 \dot{\omega}_c f(c)\, dc \longrightarrow 0 \text{ AS } C \to 0$$

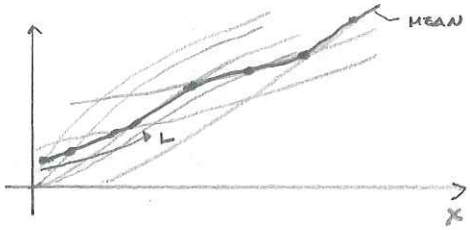
AN ALTERNATIVE METHOD FOR MODELLING $\overline{\dot{\omega}_c}$ IS TO CONSIDER THAT $\overline{\dot{\omega}_c}$ AT A GIVEN LOCATION DEPENDS MORE ON THE PASSAGE OR CROSSING FREQUENCY OF THE FLAME FRONT THAN ON THE LOCAL MEAN TEMPERATURE OR PROGRESS VARIABLE:

$$\overline{\dot{\omega}_c} = \dot{\omega}_c' f_c = \left(\begin{array}{c}\text{REACTION RATE}\\ \text{PER FLAME CROSSING}\end{array}\right) \times \left(\begin{array}{c}\text{FREQUENCY}\\ \text{OF FLAME}\\ \text{CROSSING}\end{array}\right)$$

FROM STATISTICAL ANALYSIS OF THE TELEGRAPHIC SIGNAL:

$$f_c \approx \frac{2\bar{c}(1-\bar{c})}{T} = \frac{2}{T}\frac{\tilde{c}(1-\tilde{c})(1-\alpha)}{\left[1-\alpha(1-\tilde{c})\right]^2}$$

WITH $T \sim \frac{k}{\varepsilon}$ THE MEAN PERIOD OF THE TELEGRAPHIC SIGNAL. AN EBU-LIKE EXPRESSION IS RECOVERED WHEN $\dot{\omega}_c' \sim \rho_u I_0 \Rightarrow \overline{\dot{\omega}_c} \sim 2\rho_u I_0 \frac{\varepsilon}{k}\bar{c}(1-\bar{c})$. A SPATIAL ANALOGY CAN BE CONSTRUCTED BY SUPERIMPOSING MANY TWO DIMENSIONAL REACTION PROGRESS CONTOURS. BY TRAVELLING ALONG THE MEAN CONTOUR IT IS POSSIBLE TO GENERATE A SQUARE WAVE, THIS TIME CORRESPONDING TO REACTION PROGRESS VARIABLE VERSUS DISTANCE, WITH




$$\overline{\dot{\omega}_c} = f_s w_y = \left(\begin{array}{c}\text{REACTION RATE}\\ \text{PER FLAME}\\ \text{CROSSING}\end{array}\right) \times \left(\begin{array}{c}\text{SPATIAL FREQ.}\\ \text{OF FLAME}\\ \text{CROSSING}\end{array}\right)$$

THEN $f_s \sim \frac{\overbrace{\rho}^{\text{CONSTANT}}\bar{c}(1-\bar{c})}{\ell}$ — NOTICE THAT FLAME WRINKLING SCALES HERE WITH THE INTEGRAL SCALE $\ell$.

AND $w_y \sim \frac{\rho_u S_L^0 I_0}{|\overline{\sigma_s}|}$, WITH $\overline{\sigma_s} = \overline{\cos\Theta}$ AN ORIENTATION FACTOR, AND $I_0$ IS A STRETCH-CORRECTION FACTOR.

**FLAME SURFACE-DENSITY MODELS** (MARBLE AND BROADWELL, 1977)

AN ALTERNATIVE WAY OF CLOSING $\overline{\dot{\omega}_c}$ IS TO MAKE USE OF THE FLAME-SURFACE DENSITY $\Sigma$ (FLAME SURFACE PER UNIT VOLUME) = MEASURES FRONT CONVOLUTIONS

$$\overline{\dot{\omega}_c} = \rho_u \langle S_c \rangle_s \Sigma$$ — FLAME-FRONT VISUALIZATIONS ARE REQUIRED TO DETERMINE THIS FROM EXPERIMENTS.

WITH $\langle S_c \rangle_s$ THE AVERAGE FLAME-CONSUMPTION SPEED ALONG THE SURFACE. THIS APPROACH IS VALID IN THE FLAMELET LIMIT. HERE, THE CHEMISTRY (WHICH INFLUENCES $\langle S_c \rangle_s$) IS DECOUPLED FROM FLAME-TURBULENCE INTERACTIONS (GIVEN BY $\Sigma$).

$$\frac{S_c}{S_L^0} \sim \int_{-\infty}^{+\infty} \frac{\dot{w}_F}{\rho_u S_L^0}\cdot dn$$, WITH $n$ THE LOCAL NORMAL TO THE FLAME.

IN THIS APPROACH, THE TURBULENT FLAME IS VIEWED AS AN ENSEMBLE OF FLAMELETS, WHICH USUALLY HAVE A STRUCTURE SIMILAR TO A PREMIXED LAMINAR FLAME IN A COUNTERFLOW CONFIGURATION (SEE FIG.4). THE FLAME SPEED IS CALCULATED FOR EVERY FLAMELET, INCLUDING COMPLEX CHEMISTRY, AND IS TABULATED AS A FUNCTION OF THE LOCAL STRETCH, TEMPERATURE, COMPOSITION, ETC. THE MEAN CONSUMPTION RATE IS THEN GIVEN BY:

$$\langle S_c \rangle_s = \int_0^{+\infty} S_c(\kappa) P(\kappa) d\kappa$$

WHERE $P(\kappa)$ IS THE PROBABILITY TO HAVE THE STRETCH $\kappa$ ON THE FLAME SURFACE. IN PRACTICAL IMPLEMENTATIONS, $P(\kappa) = \delta(\kappa - \bar{\kappa})$, WHERE $\bar{\kappa}$ IS THE MEAN LOCAL STRETCH RATE. THEN $\langle S_L \rangle_s \sim S_L(\bar{\kappa})$ AND $Da \sim S_L(\bar{\kappa}) / S_L^0 \sim 1$. $\rightarrow \bar{\kappa} \sim k/\varepsilon \sim \frac{1}{\tau}$ → SCALES WITH LOCAL INTEGRAL TIME SCALE

NOTICE THAT A TURBULENT FLAME SPEED MAY BE DEFINED AS $S_T \sim \langle S_c \rangle_s \Sigma / \Sigma_0$, WHICH IS FOUND TO DEPEND STRONGLY ON LEWIS NUMBER EFFECTS, WHICH TEND TO INCREASE $\Sigma$ BY DIFFUSIVE-THERMAL INSTABILITIES (HAWORTH + POINSOT, 1992). NOTICE THAT $S_L$ IS SENSITIVE TO THE LEWIS NUMBER OF THE DEFICIENT REACTANT (SEE FIG. 5).

CLOSURE FOR $\Sigma$ IS ACHIEVED EITHER BY ALGEBRAIC RELATIONS OR BY SOLVING A TRANSPORT EQUATION FOR $\Sigma$.

- ALGEBRAIC EXPRESSIONS FOR $\Sigma$: COMPARING THE CROSSING-FREQUENCY MODEL $\bar{\omega}_c = \frac{f_s \rho_u S_L^0}{|\overline{\sigma_s}|}$ WITH $\bar{\omega}_c = \rho_u S_L^0 \Sigma$, THEN $\Sigma = f_s / |\overline{\sigma_s}| = \frac{\bar{c}(1-\bar{c})}{|\overline{\sigma_s}| L}$.




- BALANCE EQUATION FOR $\Sigma$: (SEE VERVISCH ET AL, 1994 FOR FORMAL DERIVATION):

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot \left( \langle \underline{u} \rangle_s \Sigma \right) + \nabla \cdot \left( \langle S_d \rangle_s \Sigma \right) = \langle \nabla \cdot \underline{u} - \underline{n}\underline{n} : \nabla \underline{u} \rangle_s \Sigma - \langle S_d \nabla \cdot \underline{n} \rangle_s \Sigma$$

UNSTEADY EFFECTS; ADVECTION; DISPLACEMENT SPEED; TANGENTIAL STRAIN RATE; CURVATURE; STRETCH

WITH $\Sigma = \overline{|\nabla c| \delta(c - c^*)}$, DISPLACEMENT SPEED $= \frac{1}{|\nabla c|} \frac{Dc}{Dt}$

$n_i n_j \frac{\partial u_i}{\partial x_j}$

* INTERMISSION: THE LAMINAR FLAME SPEED IS TYPICALLY MODIFIED TO ACCOUNT FOR FLAME STRETCH AS: $S_L = S_L^0 - S_L^0 \mathcal{L} \mathcal{K} - \mathcal{L} \mathcal{S}$ (CURVATURE; STRAIN)

$\mathcal{K} = -\nabla \cdot \underline{n}$ CURVATURE

$\mathcal{S} = \nabla \cdot \underline{u} - \underline{n}\underline{n} : \nabla \underline{u}$ TANGENTIAL STRAIN RATE




THE FLAME STRETCH $k = \frac{1}{A} \frac{dA}{dt} = \nabla \cdot \underline{u}_F - \underline{n}\underline{n} : \nabla \underline{u}_F = \nabla \cdot \underline{v} - \underline{n}\underline{n} : \nabla \underline{v} - S_L \nabla \cdot \underline{n}$

$\underline{u}_F = \underline{v} - \underline{n} S_L$ (KINEMATIC BALANCE, PAG 17)

IS THE LAGRANGIAN TIME DERIVATIVE OF THE LOGARITHM OF AN AREA ELEMENT OF THE FLAME SHEET, AND IT IS COMPOSED OF TANGENTIAL STRAIN RATE $\mathcal{S}$ AND CURVATURE $\mathcal{K}$. THE MARKSTEIN LENGTH $\mathcal{L} = M_a \cdot \delta_L^0$ IS PROPORTIONAL TO THE FLAME THICKNESS, WITH $M_a$ A MARKSTEIN NUMBER THAT MUST BE CALCULATED BY ANALYZING THE FLAME STRUCTURE (SEE WILLIAMS + CLAVIN, 1982): $\frac{\mathcal{L}}{\delta_L^0} = \frac{1}{\alpha} \ln\left(\frac{1}{1-\alpha}\right) + \beta \frac{(Le-1)}{2} \left(\frac{1-\alpha}{\alpha}\right) \int_0^{\frac{\alpha}{1-\alpha}} \frac{\ln(1+x)}{x} dx$ WITH

$Le$ THE LEWIS NUMBER OF THE DEFICIENT REACTANT. THIS EXPRESSION, WHICH IS FOR 1-STEP CHEMISTRY AT LARGE ACTIVATION ENERGIES, HAS BEEN EXTENDED BY ROGG AND PETERS FOR A 4-STEP MECHANISM FOR $CH_4$-AIR. NEGATIVE MARKSTEIN LENGTHS CAN BE ACHIEVED WHEN

$$Le < Le_c = 1 - \frac{1}{\beta} \left[ \frac{2}{1-\alpha} \ln\left(\frac{1}{1-\alpha}\right) \right] \Big/ \int_0^{\frac{\alpha}{1-\alpha}} \frac{\ln(1+x)}{x} dx$$

NOTICE THAT $\mathcal{L} \sim \delta_L^0 \Rightarrow$ CURVATURE EFFECTS ARE IMPORTANT FOR CURVATURE RADII OF ORDER $\delta_L^0$

IN PARTICULAR, DIFFUSIVE-THERMAL INSTABILITIES OF THE CELLULAR TYPE BECOME IMPORTANT ($\rightarrow H_2$ LEAN DEFLAGRATIONS) WHEN $Le < Le_c$, WITH $Le_c \sim 0.5$ FOR MOST SITUATIONS. NOTICE THAT $Le_c \rightarrow 1 - \frac{2}{\beta}$ WHEN $\gamma \rightarrow 0$, SO THE LIMIT Le NUMBER IS 1 IN THE FIRST APPROXIMATION IN $\beta \gg 1$ AND $1 - \frac{2}{\beta}$ IN THE SECOND APPROXIMATION WHEN THERE IS NO THERMAL EXPANSION.

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THE BALANCE EQUATION FOR $\Sigma$ IS UNCLOSED AND REQUIRES MODELLING FOR THE TURBULENT FLUX, THE PROPAGATION SPEED / STRAIN RATE AND CURVATURE. WHEN THE DECOMPOSITION

$$\langle U \rangle_s = \langle \tilde{\underline{U}} + \underline{U}'' \rangle_s = \tilde{\underline{U}} + \langle U'' \rangle_s \quad \text{IS PERFORMED, THE BALANCE EQUATION}$$

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\tilde{\underline{U}} \Sigma) = - \nabla \cdot \left( \Sigma \langle \underline{U}'' \rangle_s \right) + k_m \Sigma + k_t \Sigma - \langle S_d \nabla \cdot \underline{n} \rangle_s \Sigma$$

WHERE THE PROPAGATION TERM $\nabla \cdot (\langle S_d \rangle_s \Sigma)$ HAS BEEN NEGLECTED (GOOD APPROXIMATION IF $S_L \ll U$) AND $k_m$ AND $k_t$ ARE GIVEN BY:

$k_m = \nabla \cdot \tilde{\underline{U}} - \underline{n}\underline{n} : \nabla \tilde{\underline{U}}$ INDUCED STRAIN BY THE MEAN FLOW

$k_t = \langle \nabla \cdot \underline{U}'' - \underline{n}\underline{n} : \nabla \underline{U}'' \rangle_s$ " " BY THE TURBULENT MOTIONS

THIS EQUATION CAN BE REWRITEN AS:

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\tilde{\underline{U}} \Sigma) = \underbrace{\nabla \cdot \left( \frac{\nu_t}{\sigma_\Sigma} \nabla \Sigma \right)}_{①} + \underbrace{k_m \Sigma + k_t \Sigma}_{②} - \underbrace{D}_{③}$$

WHERE THE ASSUMPTION $\langle U'' \rangle_s \Sigma = - \frac{\nu_t}{\sigma_\Sigma} \nabla \Sigma$ HAS BEEN MADE, WITH $\nu_t$ THE EDDY VISCOSITY AND $\sigma_\Sigma$ A TURBULENT SCHMIDT #.

→ NOTICE THAT A COUNTERGRADIENT TRANSPORT IS OBSERVED IN $\Sigma$ AS WELL (PAGE 284 VEYNANTE & VERVISCH 2002)

TERM ① REFERS TO THE TURBULENT TRANSPORT OF $\Sigma$, TERMS ② ARE PRODUCTION TERMS OF FLAME SURFACE DENSITY BECAUSE OF STRAIN, AND TERM ③ IS A SINK OF $\Sigma$.

THE DISPLACEMENT TERM D ACTS TO DECREASE THE FLAME SURFACE GROWTH, WHICH OTHERWISE WOULD GROW CONTINUOUSLY BECAUSE OF STRETCH $k_m$ AND $k_t$ IN ANALOGY WITH NON REACTING MATERIAL SURFACES.

WHEN THE STRAIN RATE TERM IS APPROXIMATED AS $k_m \Sigma + k_t \Sigma \sim \alpha_0 \frac{\varepsilon}{k} \Sigma$ ($\frac{k}{\varepsilon}$: INTEGRAL TIME SCALE) AND THE DESTRUCTION TERM D IS SIMPLIFIED TO BE PROPORTIONAL TO THE MEAN REACTION RATE AND INVERSELY PROPORTIONAL TO THE AVAILABLE REACTANTS PER UNIT FLAME AREA $\left( \frac{1-\tilde{c}}{\Sigma} \right)$, $D \sim \beta_0 \langle S_c \rangle_s \frac{\Sigma^2}{1-\tilde{c}}$

THEN ONE OBTAINS:

$$\boxed{\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\tilde{\underline{U}} \cdot \Sigma) = \nabla \cdot \left( \frac{\nu_t}{\sigma_\Sigma} \nabla \Sigma \right) + \alpha_0 \frac{\varepsilon}{k} \Sigma - \beta_0 \langle S_c \rangle_s \frac{\Sigma^2}{1-\tilde{c}}}$$

$\alpha_0, \beta_0$ CONSTANTS

WHEN $\Sigma$ IS IN DYNAMICAL EQUILIBRIUM (PRODUCTION = DESTRUCTION), THEN

$$\alpha_0 \frac{\varepsilon}{k} = \beta_0 \langle S_c \rangle_s \frac{\Sigma}{1-\tilde{c}}, \quad \text{AND FROM THE DEFINITION OF } \bar{\dot{\omega}}_c:$$

$$\bar{\dot{\omega}}_c = \rho_u \langle S_c \rangle_s \Sigma, \quad \text{THEN} \quad \boxed{\bar{\dot{\omega}}_c = \rho_u \frac{\alpha_0}{\beta_0} \frac{\varepsilon}{k} (1 - \tilde{c})} \quad \text{(EBU-LIKE CLOSURE)}$$

⇒ IN DYNAMICAL EQUILIBRIUM FOR $\Sigma$, THE MEAN REACTION RATE IS "INDEPENDENT" OF CHEMISTRY AND AN EBU-TYPE OF SOLUTION (INFINITELY-FAST CHEMISTRY LIMIT) IS OBTAINED.

⇒ OVERALL PROBLEM: CONTINUITY + MOMENTUM + $k$-$\varepsilon$ + PROGRESS VARIABLE EQ + SURFACE DENSITY EQ + TABLE.

## THE LEVEL-SET APPROACH (PETERS, 2000)

IN THIS APPROACH, THE FLAME FRONT IS DESCRIBED AS A GEOMETRICAL ENTITY, AND IT IS GENERALLY ASSUMED TO BE A THIN INTERFACE SEPARATING BURNT FROM FRESH GASES.

OVERALL PROBLEM: CONTINUITY + MOMENTUM + $K$-$\varepsilon$ EQUATIONS + TRANSPORT EQ FOR $\tilde{G}$ +
+ TRANSPORT EQUATION FOR $\tilde{G}''^2$ + TRANSPORT EQ. FOR $\bar{\sigma} = |\overline{\nabla G}|$ +
+ TABLE TO OBTAIN $\tilde{\gamma}_i$ AND $\bar{\rho}$ USING PRESUMED PDF.

$G$: LEVEL-SET FUNCTION

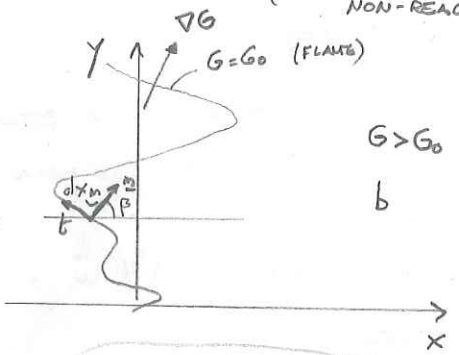
⇒ "$G$-BASED FLAMELET APPROACH" FOR TURBULENT FLAME PROPAGATION.

FLAMELET MODELS ASSUME SCALE SEPARATION BETWEEN THE SMALL SCALES AT WHICH CHEMICAL REACTION OCCUR AND THE LARGER SCALES IN THE INERTIAL RANGE. SINCE MIXING IS MODELLED BY USING INERTIAL-RANGE INVARIANT DISSIPATION RATES, FLAMELETS DO NOT INTRODUCE A REYNOLDS-NUMBER DEPENDENCE IN THE LARGE REYNOLDS LIMIT.

THE ADVANTAGES OF USING THE LEVEL-SET FUNCTION OVER OTHER APPROACHES ARE:

i) NO NEED TO DEAL WITH COUNTERGRADIENT DIFFUSION SINCE THE TURBULENT FLUXES NORMAL TO THE FLAME FRONT DO NOT APPEAR IN THE FORMULATION.

ii) NO NEED FOR CHEMICAL-SOURCE CLOSURE SINCE THE LEVEL-SET FUNCTION $G$ IS A NON-REACTING SCALAR.




IF $G(\underline{x},t) = G_0$ DENOTES THE SURFACE OF THE FLAME, THEN

$$\frac{\partial G}{\partial t} + \underline{U}_F \cdot \nabla G = 0,$$

WITH $\underline{U}_F = \underline{v} - S_L \cdot \underline{n}$ THE ABSOLUTE PROPAGATION VELOCITY OF THE FRONT. SUBSTITUTING THIS KINEMATIC RELATION IN THE EQUATION ABOVE, ONE OBTAINS THE $G$-EQUATION:

$$\boxed{\frac{\partial G}{\partial t} + \underline{v} \cdot \nabla G = S_L |\nabla G|} \quad \text{(WILLIAMS, 1985)}$$

SUPPLIED WITH REINITIALIZATION $|\nabla G| = 1$ OUTSIDE $G = G_0$ TO AVOID UNPHYSICAL FEEDBACK FROM THE 3D $G$ FIELD

NOTICE THAT THIS IS CONSTANT $\rho$. IF $\rho$ IS NOT CONSTANT AND $S_L = S_L^u \rightarrow \underline{v}$ IS CONDITIONED ON THE UNBURNT AND SIDE AND $\frac{\rho_u}{\rho_b}$

THIS EQUATION IS APPLICABLE TO THIN FLAMES THAT PROPAGATE WITH A WELL-DEFINED VELOCITY $S_L$, WITH A FLAME THICKNESS SMALLER THAN THE KOLMOGOROV SCALE → CORRUGATED AND WRINKLED FLAMELET REGIME. THEREFORE, THE ENTIRE FLAME STRUCTURE REMAINS EMBEDDED IN A QUASI-LAMINAR FLOW FIELD AND THE LAMINAR BURNING VELOCITY REMAINS WELL DEFINED. THE $G$-EQUATION DOES NOT CONTAIN ANY DIFFUSION-LIKE TERM IF $S_L$ IS JUST A SCALAR INDEPENDENT OF STRETCH. THE QUANTITY $G$ IS A SCALAR DEFINED AT THE SURFACE ONLY, WHILE THE SURROUNDING $G$ FIELD IS NOT UNIQUELY DEFINED. THIS IS BECAUSE WHILE THE KINEMATIC BALANCE $\underline{U}_F = \underline{v} - S_L \cdot \underline{n}$ DESCRIBES A TWO-DIMENSIONAL SURFACE, THE $G$-EQUATION IS AN EQUATION IN THREE DIMENSIONS. THE LEVEL-SET FUNCTION THUS DIFFERS FROM THE MIXTURE FRACTION $Z$ TYPICALLY USED IN NON-PREMIXED COMBUSTION, WHICH IS A CONSERVED SCALAR THAT IS WELL DEFINED EVERYWHERE.

THE DISTANCE $x_m$ FROM THE FLAME SURFACE IN THE NORMAL DIRECTION (TOWARDS THE BURNT SIDE) IS

$$dx_m = \underline{n} \cdot d\underline{x} = \frac{\nabla G}{|\nabla G|} \cdot d\underline{x} = \frac{dG}{\sigma}, \quad \text{WITH } \sigma = |\nabla G|$$

AVOIDS THE PRESENCE OF FLAME CUSPS

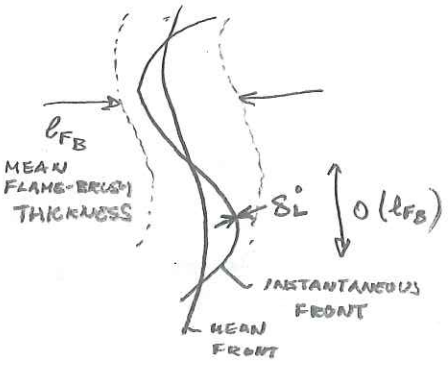
SINCE $G$ IS NOT UNIQUELY DEFINED OUTSIDE $G(\underline{x},t) = G_0$, THE FLAMELET FORMULATION USES $x_m$, WHICH RESOLVES THE DISTANCE NORMAL TO THE INSTANTANEOUS FLAME SURFACE.

WHEN THE CURVATURE CORRECTION IS CONSIDERED FOR THE PROPAGATION SPEED (SEE PAGE 11), THE $G$-EQUATION BECOMES ⇒ $\frac{\partial G}{\partial t} + \underline{v} \cdot \nabla G = S_L^0 |\nabla G| - D_M \mathcal{K} |\nabla G|$, WITH $D_M = \mathcal{L} S_L^0$ A MARKSTEIN DIFFUSIVITY.

$\mathcal{K} = -\nabla \cdot \underline{n} + \underline{n} \cdot \nabla |\nabla G| / |\nabla G|$ ⇒ FOR $D_M > 0$, THE CURVATURE TERM ADDS A DIFFUSION-LIKE OPERATOR: $\mathcal{K} = -\nabla \cdot \underline{n} = -\nabla \cdot \left( \frac{\nabla G}{|\nabla G|} \right)$ (20)

## THE FLAMELET ASYMPTOTIC LIMIT (PREMIXED)

IN THIS LIMIT, THE CHARACTERISTIC LENGTH ASSOCIATED WITH THE CORRUGATIONS OF THE FLAME, $\Lambda \sim \frac{(\widetilde{G''^2})^{1/2}}{\sigma}$, IS MUCH LARGER THAN THE FLAME THICKNESS $\delta_L^0$, WITH $\varepsilon = \frac{\delta_L^0 \sigma}{(\widetilde{G''^2})^{1/2}} \ll 1$ A SMALL PARAMETER, WITH $\sigma = O(1)$. IF $P(G; \underline{x}, t)$ IS THE PDF FOR THE SCALAR $G$, THEN




THE PROBABILITY DENSITY FUNCTION OF FINDING THE FLAME SURFACE IS $P(\underline{x}, t) = \int_{-\infty}^{+\infty} \delta(G - G_0) P(G; \underline{x}, t)\, dG$ (SEE FIG 6)

THE FLAMELET LIMIT, $\varepsilon = \frac{\delta_L}{\Lambda} \ll 1$, $\Lambda \sim l_{F,B}$

THIS PDF CAN BE MEASURED BY COUNTING THE NUMBER OF FLAME CROSSINGS IN A SMALL VOLUME CENTERED AT $\underline{x}$ DURING A SMALL TIME INTERVAL. THE MEAN FLAME POSITION AND MEAN FLAME BRUSH THICKNESS ARE $\overline{x_f} = \int_{-\infty}^{+\infty} x P(x)\, dx$ AND $l_{F_B} = \overline{(x - \overline{x_f})^2}^{1/2}$ RESPECTIVELY. WHEN A LINEAR DEPENDENCE OF $G$ ON $x$ IS CHOSEN, $\overline{G}(x) - G_0 = x - \overline{x_f}$, THEN $G' = G - \overline{G} = G_0 - G - (x - \overline{x_f})$, WHICH AT THE FRONT BECOMES $G' = -(x - \overline{x_f}) \Rightarrow \boxed{(\overline{G'^2})^{1/2} = l_{F_B}}$,

OR EQUIVALENTLY, "THE FLUCTUATIONS OF $G$ AT THE FLAME REPRESENT THE SCALAR DISTANCE BETWEEN THE MEAN AND THE INSTANTANEOUS FLAME FRONT MEASURED IN THE DIRECTION NORMAL TO THE MEAN TURBULENT FLAME".

CONSIDER THE SPECIES CONSERVATION EQUATION $\rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla Y_i = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{w}_i$.

WHEN THIS EQUATION IS WRITTEN IN TERMS OF THE DIMENSIONLESS VARIABLES

$\underline{x}^* = \underline{x}/\Lambda$, $t^* = t \delta_L^0/\Lambda$, $\underline{v}^* = \underline{v}/\delta_L^0$, $\rho^* = \rho/\rho_0$, $\dot{w}_i^* = \frac{\dot{w}_i \delta_L^0}{\delta_L^0 \rho_0}$, $D_i^* = \frac{D}{\delta_L^0 \delta_L}$

ONE OBTAINS $\rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla Y_i = \varepsilon \nabla \cdot (\rho D_i \nabla Y_i) + \frac{\dot{w}_i}{\varepsilon}$ WHERE THE * HAS BEEN DROPPED.

SINCE $dx_n = \frac{dG}{\sigma} \Rightarrow$ AT THE FLAME $\delta_L \sim \frac{\Delta G}{\sigma} \rightarrow \frac{\Delta G}{(\widetilde{G''^2})^{1/2}} \sim \frac{\delta_L \sigma}{(\widetilde{G''^2})^{1/2}} = \varepsilon \ll 1$

IN PARTICULAR, AN "INNER" LEVEL SET FUNCTION IS DEFINED AS $\mathcal{G} = \frac{(G - G_0)/(\widetilde{G''^2})^{1/2}}{\varepsilon}$ WITH $\mathcal{G} \sim O(1)$ IN THE FLAME. BY TAKING $Y_i = Y_i(\hat{G}, \underline{x}_\perp, t)$, WITH $\underline{x}_\perp$ THE SET OF COORDINATES TANGENTIAL TO THE FRONT AND $\hat{G} = \frac{G - G_0}{(\widetilde{G''^2})^{1/2}}$, THEN

$$\left.\begin{aligned} \frac{\partial}{\partial t} &= \frac{\partial \hat{G}}{\partial t}\frac{\partial}{\partial \hat{G}} + \frac{\partial}{\partial t} \\ \nabla &= \nabla \hat{G}\frac{\partial}{\partial \hat{G}} + \nabla_\perp \end{aligned}\right\} \Rightarrow \text{THE SPECIES EQUATION BECOMES:}$$

$$\left[\rho \frac{\partial \hat{G}}{\partial t} + \rho \underline{v} \cdot \nabla \hat{G}\right]\frac{\partial Y_i}{\partial \hat{G}} + \rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla_\perp Y_i = \varepsilon \nabla \hat{G} \frac{\partial}{\partial \hat{G}}\left(\rho D_i \nabla \hat{G} \frac{\partial Y_i}{\partial \hat{G}}\right)$$
$$+ \varepsilon \nabla \hat{G} \frac{\partial}{\partial G}\left(\rho D_i \nabla_\perp Y_i\right) + \varepsilon \nabla_\perp \cdot \left(\rho D_i \nabla_\perp Y_i\right) + \varepsilon \nabla_\perp \cdot \left(\rho D_i \nabla \hat{G} \frac{\partial Y_i}{\partial \hat{G}}\right) + \frac{\dot{w}_i}{\varepsilon}.$$

INTRODUCING THE INNER LEVEL SET $\mathcal{G}$ IN THE EQUATION ABOVE, ONE OBTAINS:

$$\frac{1}{\varepsilon}\left[\rho \frac{\partial \hat{G}}{\partial t} + \rho \underline{v} \cdot \nabla \hat{G}\right]\frac{\partial Y_i}{\partial \mathcal{G}} + \rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla_\perp Y_i = \frac{1}{\varepsilon} \nabla \hat{G} \frac{\partial}{\partial \mathcal{G}}\left(\rho D_i \nabla \hat{G} \frac{\partial Y_i}{\partial \mathcal{G}}\right) + \nabla \hat{G} \frac{\partial}{\partial \mathcal{G}}\left(\rho D_i \nabla_\perp Y_i\right) +$$
$$+ \varepsilon \nabla_\perp \cdot \left(\rho D_i \nabla_\perp Y_i\right) + \nabla_\perp \cdot \left(\rho D_i \nabla \hat{G} \frac{\partial Y_i}{\partial \mathcal{G}}\right) + \frac{\dot{w}_i}{\varepsilon};$$

SINCE $\rho \frac{\partial \hat{G}}{\partial t} + \rho \underline{v} \cdot \nabla \hat{G} = |\nabla \hat{G}| = O(1)$, THEN, THE DOMINANT BALANCE IN THE PREVIOUS

EQUATION IS: $$\left[\rho\frac{\partial\hat{G}}{\partial t}+\rho\underline{v}\cdot\nabla\hat{G}\right]\frac{\partial Y_i}{\partial\theta_\gamma}=\nabla\hat{G}\frac{\partial}{\partial\theta_\gamma}\left(\rho D_i\nabla\hat{G}\frac{\partial Y_i}{\partial\theta_\gamma}\right)+\dot{W}_i,\quad \text{TO ORDER } \frac{1}{\varepsilon},$$

WHICH IN THE ORIGINAL DIMENSIONAL VARIABLES BECOMES

$$\boxed{\rho S_L^0\sigma\frac{\partial Y_i}{\partial G}=\frac{\partial}{\partial G}\left(\rho D_i\sigma^2\frac{\partial Y_i}{\partial G}\right)+\dot{W}_i}$$

→ SIMILAR TO NON-PREMIXED COMBUSTION ($G\to Z$, $\sigma\to\chi$)

IN WHICH $G$ IS THE INDEPENDENT VARIABLE AND $\sigma=|\nabla G|$ IS A PARAMETER THAT VARIES IN SCALES MUCH LONGER THAN $\varepsilon G$. A SPATIAL ANALOGY CAN BE OBTAINED FOR $\frac{X_M-X_{M_f}}{\delta_L^0}\sim O(1)$ SUCH THAT $\sigma$ IS CONSTANT ALONG DISTANCES OF $O(\delta_L)$ NORMAL TO THE FLAME AND THE EQUATION ABOVE BECOMES

$$\boxed{\rho S_L^0\frac{\partial Y_i}{\partial x_m}=\frac{\partial}{\partial x_m}\left(\rho D_i\frac{\partial Y_i}{\partial x_m}\right)+\dot{W}_i}$$

STEADY PREMIXED-FLAMELET EQUATION. ($S_L^0$ = EIGENVALUE)

NOTICE THAT:

i) UNSTEADY EFFECTS HAVE BEEN ASSUMED TO OCCUR IN LONG SCALES (OF ORDER $\frac{\ell_{FB}}{S_L^0}$). THEY WOULD APPEAR IN THE FLAMELET EQUATION IF THEY HAPPENED OVER TIME SCALES OF ORDER $\delta_L^0/S_L^0$ (i.e. $\varepsilon$ TIMES SHORTER THAN $\ell_{FB}/S_L^0$).

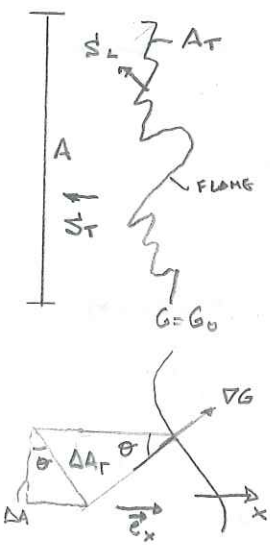
ii) FLAME-STRETCH EFFECTS HAVE NOT BEEN CONSIDERED HERE, SINCE THE THE SCALING OF THE TANGENTIAL COORDINATES GOES LIKE $\ell_{FB}$ IN THE ANALYSIS ABOVE. ONE WOULD NEED FLAME WRINKLES OF LENGTHS OF ORDER $\delta_L^0$ IN ORDER TO RETAIN THE EFFECTS OF CURVATURE AND STRAIN IN THE ANALYSIS ABOVE.

MARKSTEIN NUMBER $M_a=\frac{\mathcal{L}}{\delta_L}\sim 1$

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INTERMISSION: THE TURBULENT BURNING VELOCITY (DAMKÖHLER, 1940)

DAMKÖHLER WAS THE FIRST WHO OBTAINED EXPRESSIONS FOR THE TURBULENT BURNING VELOCITY IN WHAT HE CALLED "LARGE-SCALE" TURBULENCE (i.e. THE INTERACTION BETWEEN FLAME AND TURBULENCE IS PURELY KINEMATIC → CORRUGATED FLAMELETS) AND "SMALL-SCALE" TURBULENCE (i.e. TURBULENCE MODIFIES THE TRANSPORT BETWEEN THE REACTION ZONE AND THE UNBURNT GAS → THIN-REACTION S). DAMKÖHLER EQUATED THE MASS FLUX $\dot{m}$ OF UNBURNT GAS WITH THE LAMINAR BURNING VELOCITY $S_L$ THROUGH THE TURBULENT (CORRUGATED) FLAME AREA $A_T$, TO THE MASS FLUX THROUGH THE CROSS-SECTIONAL AREA $A$ WITH THE TURBULENT BURNING VELOCITY $S_T$




$$\dot{m}=\rho_u S_L A_T=\rho_u S_T A\ \Rightarrow\ \frac{S_T}{S_L}=\frac{A_T}{A}.$$

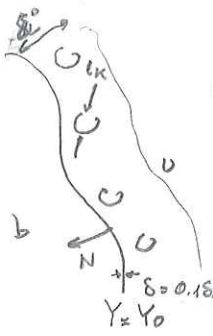
IN GENERAL, IT IS ASSUMED THAT $\frac{S_T}{S_L}\sim\left(1+C\left(\frac{u'}{S_L}\right)^n\right)^{1/m}$, ALTHOUGH EXPRESSIONS OF THIS TYPE CAN BE DERIVED UNDER SOME APPROXIMATIONS (SEE, FOR INSTANCE, WILLIAMS' COMBUSTION THEORY, PAGE 429). IN THE LIMIT $\frac{u'}{S_L}\gg 1$, THEN $\frac{S_T}{S_L}\sim\frac{u'}{S_L}\Rightarrow S_T\sim u'$. ALSO $S_L\sim\left(D/t_c\right)^{1/2}$, BUT $S_T\sim\left(D_t/t_c\right)^{1/2}$ (EDDY DIF.) $\to\frac{S_T}{S_L}\sim\left(\frac{D_t}{D}\right)^{1/2}\sim\left(\frac{u'}{S_L}\frac{\ell}{\ell_F}\right)^{1/2}\sim Re_t^{1/2}$ FOR $u'/S_L\gg 1$ IN SMALL-SCALE TURBULENCE. (NOTICE THAT ACCORDING TO THIS ARGUMENT, $t_c$ IS NOT AFFECTED BY TURBULENCE).




⇒ LARGE-SCALE TURBULENCE: $S_T/S_L\sim 1+u'/S_L\to S_T\sim u'$ FOR $u'/S_L\gg 1$ $\left(\text{STILL }\frac{\ell_x}{\ell_F}\ll 1\right)$

⇒ SMALL-SCALE TURBULENCE: $S_T/S_L\sim\left(D_t/D\right)^{1/2}$ $\left(\frac{l_x}{\ell_F}<1\right)$

NOTICE THAT $\frac{\Delta A_T}{\Delta A}=\left(\frac{|\nabla G|}{|\underline{e}_x\cdot\nabla G|}\right)_0$, WITH $\left(\frac{|\nabla G|}{|\underline{e}_x\cdot\nabla G|}\right)_0=\lim_{A\to\infty}\frac{1}{A}\int\frac{|\nabla G|_0}{|\underline{e}_x\cdot\nabla G|_0}\,dA$; BUT IF FLAME DOES NOT FOLD BACK, THEN $G=x-F(y,z,t)$ AND $\overline{\sigma}=\overline{|\nabla G|}=\frac{1}{\langle|\underline{e}_x\cdot\nabla G|\rangle_0}$ (21)




$\underline{n} = -\dfrac{\nabla Y}{|\nabla Y|}$

Y COULD BE, FOR INSTANCE, THE PROGRESS VARIABLE C

A LEVEL-SET FORMULATION CAN BE DERIVED FOR THE THIN REACTIONS REGIME BY CONSIDERING ISO-SCALAR SURFACES OF, FOR INSTANCE, MASS FRACTIONS ($Y_F$ FOR $\phi<1$ OR $Y_{O_2}$ FOR $\phi>1$). (SEE PETERS, 1999, JFM)

FROM THE SPECIES CONSERVATION EQUATION:

$$\rho\left(\frac{\partial Y}{\partial t} + \underline{v}\cdot\nabla Y\right) = \nabla\cdot(\rho D\nabla Y) + \dot{w}$$

THE ISO-SCALAR SURFACE OF $Y$ MUST SATISFY THE EQUATION: $\dfrac{\partial Y}{\partial t} + \underline{U}_F\cdot\nabla Y = 0$.

SINCE $\underline{U}_F = \underline{v} - S_L^0\,\underline{n}$, THEN, THIS EQUATION BECOMES $\dfrac{\partial Y}{\partial t} + \underline{v}\cdot\nabla Y = S_d|\nabla Y|$, AND WHEN COMPARISON IS MADE WITH THE SPECIES EQUATION, A DISPLACEMENT VELOCITY (GIBSON, 1968)

$$S_d = \left[\frac{\nabla\cdot(\rho D\nabla Y) + \dot{w}}{\rho|\nabla Y|}\right]_{FRONT}$$

CAN BE DEFINED. NOTICE THAT

$$\rightarrow\quad S_d = \frac{1}{|\nabla Y|}\cdot\left.\frac{DY}{Dt}\right|_{FRONT}$$

$$\nabla\cdot(\rho D\nabla Y)_{FRONT} = -\rho D|\nabla Y|\nabla\cdot\underline{n} - \rho D\,\underline{n}\cdot\nabla(|\nabla Y|) - \underline{n}|\nabla Y|\cdot\nabla(\rho D) =$$

$$= -\rho D|\nabla Y|\nabla\cdot\underline{n} + \underline{n}\cdot\nabla(\rho D\,\underline{n}\cdot\nabla Y)\ ,\quad \text{AND THEREFORE}$$

$$S_d = -\frac{\rho D|\nabla Y|\nabla\cdot\underline{n}}{\rho|\nabla Y|} + \frac{\underline{n}\cdot\nabla(\rho D\,\underline{n}\cdot\nabla Y)}{\rho|\nabla Y|} + \frac{\dot{w}}{\rho|\nabla Y|} = \underbrace{-D\mathcal{K}}_{\text{CURVATURE}} + \underbrace{S_m}_{\text{DIFFUSION NORMAL TO INTERFACE}} + \underbrace{S_r}_{\text{CHEMICAL REACTION}}$$

IN STEADY, UNSTRETCHED FLAMES, $S_m + S_r = S_L^0$. HOWEVER, IN THE THIN REACTIONS REGIME, THE UNSTEADY MIXING AND DIFFUSION OF ALL CHEMICAL SPECIES AND THE TEMPERATURE IN THE REGIONS AHEAD OF THE THIN REACTION ZONE WILL INFLUENCE THE LOCAL DISPLACEMENT SPEED. THEN, $S_m + S_r \neq S_L^0$, AND $S_d$ BECOMES A FLUCTUATING QUANTITY THAT COUPLES THE G-EQUATION TO THE SOLUTION OF THE BALANCE EQUATIONS FOR THE SCALARS. NONETHELESS, $S_m + S_m = O(S_L^0)$. BY IDENTIFYING THE $Y = Y_0$ ISOCONTOUR WITH $G = G_0$, A G EQUATION FOR THE THIN REACTIONS REGIME

$$\rho\frac{\partial G}{\partial t} + \rho\underline{v}\cdot\nabla G = -\rho D\mathcal{K}\sigma + \rho S_L^{**}\sigma \qquad (\text{"DIFFUSIVE" G-EQUATION})$$

CAN BE OBTAINED, WITH $\sigma = |\nabla G|_0$ AND $S_L^{**} = S_m + S_r$. NOTICE THAT $D$ IS NOT $D_{\mathcal{K}}$ BUT THE MOLECULAR DIFFUSIVITY, ($D>0$ ALWAYS BUT $D_{\mathcal{K}}<0$ FOR $Le<Le_c$). JOULIN (1994) HAS SHOWN THAT IN FLAMES SUBJECT TO HIGH-FREQUENCY PERTURBATIONS ($\tau_K$ LARGE) OF TIME-DEPENDENT STRETCH, THE EFFECT OF THE TANGENTIAL STRETCH DISSAPEARS COMPLETELY AND LEWIS NUMBERS EFFECTS ALSO DISSAPEAR IN THE CURVATURE TERM, SUCH THAT $D_{\mathcal{K}} \to D$, WHICH JUSTIFIES THE FORM OF THE "DIFFUSIVE" G EQUATION.

THEN:

$$\begin{cases} \rho\dfrac{\partial G}{\partial t} + \rho\underline{v}\cdot\nabla G = \rho S_L^0\sigma - \rho D_{\mathcal{K}}\mathcal{K}\sigma - \rho\mathcal{K}\mathcal{S}\sigma & \text{FOR CORRUGATED FLAMELETS } (*) \\ \rho\dfrac{\partial G}{\partial t} + \rho\underline{v}\cdot\nabla G = -\rho D\mathcal{K}\sigma + \rho S_L^{**}\sigma & \text{FOR THIN REACTIONS } (**) \end{cases}$$

WHEN $\tau = t/\tau_K$, $\underline{x}' = \dfrac{\underline{x}}{l_K}$, $\mathcal{K}' = \mathcal{K}l_K$, $\mathcal{S}' = \mathcal{S}\tau_K$ ARE TAKEN TO NONDIMENSIONALIZE (*), THE EQUATION $\dfrac{\partial G}{\partial\tau} + \underline{v}\cdot\nabla G = \dfrac{S_L^0}{v_K}|\nabla G| - \dfrac{D_{\mathcal{K}}}{\mathcal{V}}\mathcal{K}|\nabla G| - \dfrac{\mathcal{K}}{l_K}\mathcal{S}|\nabla G|$ IS OBTAINED (DROPPED TILDES HERE)

IN NONDIMENSIONAL VARIABLES. SINCE $S_L^0/v_K \gg 1$, $\mathcal{K} \sim l_F < l_K$ AND $\dfrac{D_{\mathcal{K}}}{\mathcal{V}} \sim \dfrac{S_L^0\mathcal{K}}{\mathcal{V}} \sim \dfrac{S_L^0 l_F}{\mathcal{V}} \sim 1$ IN THE CORRUGATED FLAMELETS, THE DOMINANT TERM ON THE RIGHT HAND SIDE OF (*) IS THE PLANAR PROPAGATION TERM $\rho S_L^0\sigma$.

SIMILARLY, WHEN $\tau = t/\tau_k$, $\underline{x}' = \underline{x}/l_K$, $\mathcal{K}' = \mathcal{K} l_K$, ARE TAKEN TO NONDIMENSIONALIZE (##), THE EQUATION ON $\frac{\partial G}{\partial \tau} + \underline{v}\cdot\nabla G = \frac{S_L^*}{v_k}|\nabla G| - \frac{D}{\nu}\mathcal{K}\sigma$ IS OBTAINED IN NONDIMENSIONAL VARIABLES. SINCE $S_L^* \sim S_L << v_K$ AND $D/\nu \sim 1$, THEN THE DOMINANT TERM ON THE RIGHT HAND SIDE OF (##) IS THE CURVATURE TERM $-\frac{1}{Re}\mathcal{K}\sigma$. THIS ANALYSIS IMPLIES THAT:

i) IN THE CORRUGATED FLAMELETS, THE QUASI-PLANAR PROPAGATION OF $G$ ISO-LEVELS IN THE NORMAL DIRECTION DOMINATES, FOLLOWED BY LEWIS-NUMBER-DEPENDENT CURVATURE CORRECTIONS, FOLLOWED BY LEWIS-NUMBER-DEPENDENT TANGENTIAL STRAIN CORRECTIONS.

ii) IN THE THIN REACTION REGIMES, LEWIS-NUMBER-INDEPENDENT CURVATURE EFFECTS DOMINATE, FOLLOWED BY THE NORMAL-DIFFUSION AND REACTION-DRIVEN PROPAGATION OF THE $G$ ISO SURFACE IN THE NORMAL DIRECTION, WITH THE EFFECTS OF STRAIN DISSAPEARING.

THEREFORE, AN APPROXIMATE EQUATION VALID IN BOTH REGIMES COULD BE

$$\rho\frac{\partial G}{\partial t} + \rho\underline{v}\cdot\nabla G = \rho S_L^0\sigma - \rho D\mathcal{K}\sigma .$$

WHEN $G = \tilde{G} + G''$ AND $\underline{v} = \tilde{\underline{v}} + \underline{v}''$, THEN AN EQUATION FOR THE FAVRE AVERAGE OF $G$

$$\bar{\rho}\frac{\partial \tilde{G}}{\partial t} + \rho\underline{v}\cdot\nabla\tilde{G} = -\nabla\cdot\left(\bar{\rho}\widetilde{\underline{v}''G''}\right) + \bar{\rho}S_L^0\tilde{\sigma} - \bar{\rho}D\widetilde{\mathcal{K}\sigma} \quad , \text{ AND}$$

FOR THE FAVRE VARIANCE OF $G$, $\mathbb{K} = \nabla\cdot\left(-\frac{\nabla G}{|\nabla G|}\right)$

$$\bar{\rho}\frac{\partial}{\partial t}\left(\widetilde{G''^2}\right) + \bar{\rho}\tilde{\underline{v}}\cdot\nabla\widetilde{G''^2} = -\nabla\cdot\left(\bar{\rho}\widetilde{\underline{v}''G''^2}\right) - 2\bar{\rho}\widetilde{\underline{v}''G''}\cdot\nabla\tilde{G} - \bar{\rho}\tilde{\omega} - \bar{\rho}\tilde{\chi} - \bar{\rho}D\widetilde{\mathbb{K}\sigma}.$$

THE CONDITION $\tilde{G} = G_0$ DEFINES THE LOCATION OF THE MEAN FLAME FRONT AND $\widetilde{G''^2}$ ACCOUNTS FOR FLAME FRONT FLUCTUATIONS AND THEREFORE IT IS A MEASURE OF THE FLAME BRUSH THICKNESS. IN THESE EQUATIONS, $\tilde{\sigma}$, $\widetilde{\mathcal{K}\sigma}$, $\widetilde{\underline{v}''G''}$, $\widetilde{v''G''^2}$, $\tilde{\omega}$, $\tilde{\chi}$ AND $\widetilde{\mathbb{K}\sigma}$ NEED CLOSURE BY MODELLING.

- KINEMATIC RESTORATION: $\tilde{\omega} = -2S_L^0\widetilde{G''\sigma}$ ⇒ IT ACCOUNTS FOR THE SMOOTHING OF THE SCALAR FIELD AND FLAME SURFACE BY LAMINAR FLAME PROPAGATION. SCALAR FLUCTUATIONS OF $G$ PRODUCED BY TURBULENCE ARE RESTORED BY THIS KINEMATIC EFFECT, WHICH PLAYS A SIMILAR ROLE AS THE SCALAR DISSIPATION PLAYS FOR FLUCTUATIONS OF DIFFUSIVE SCALARS. IT IS IMPORTANT IN THE CORRUGATED FLAMELETS, IN WHICH IT IS TYPICALLY MODELLED AS $\tilde{\omega} = C_\omega\widetilde{G''^2}/T$, WITH $T = k/\varepsilon$. NOTICE THAT, SINCE $l \sim \left(\widetilde{G''^2}\right)^{1/2} \rightarrow S_L^0\tilde{\sigma}l \sim l^2/T \rightarrow \tilde{\sigma} \sim u'/S_L$, SO THAT $S_T/S_L \sim u'/S_L$. THE KINEMATIC RESTORATION IS MOST ACTIVE AT THE GIBSON SCALE $l_G$, WHICH REPRESENTS A CUTOFF LENGTH FROM THE INERTIAL RANGE IN THE SCALAR SPECTRUM FUNCTION OF $G$ (FOR $l < l_G$ $G$ CEASES TO FLUCTUATE BECAUSE OF THE KINEMATIC RESTORATION).

CORRUGATIONS PRODUCED BY TURBULENCE WOULD INCREASE EXPONENTIALLY THE AREA OF A NON-DIFFUSIVE SCALAR SURFACE WITH TIME IF IT WASN'T FOR $\tilde{\omega}$

$l_G > l_B > l$ IN THE CORRUGATED FLAMELETS.

- SCALAR DISSIPATION: $\tilde{\chi} = 2D\left(\nabla\widetilde{G''}\right)^2$ ⇒ IT IS THE DOMINANT SINK OF SCALAR FLUCTUATIONS IN THE THIN REACTIONS REGIMES. IT IS USUALLY MODELLED AS $\tilde{\chi} = C_\chi\widetilde{G''^2}/T$, WHICH SHOWS THAT, IN THE THIN REACTION REGIME, $\tilde{\chi} \sim D\tilde{\sigma}^2 \sim l^2/T \rightarrow \tilde{\sigma} \sim \left(\frac{D_t}{D}\right)^{1/2} \sim Re_t^{1/2} \sim \left(\frac{l}{l_\lambda}\right)$ WHERE $l_\lambda \sim \frac{\left(\widetilde{G''^2}\right)^{1/2}}{\tilde{\sigma}} \sim u'l_K$ IS A TAYLOR LENGTH. ⇒ $\frac{A_T}{A} \sim (Re_t)^{1/2} >> 1$.

⇒ NOTE THAT $\sigma = \int_{-\infty}^{+\infty}\Sigma\, dx_n$ WITH $\Sigma$ THE FLAME-SURFACE DENSITY.

- TURBULENT TRANSPORT TERMS: $-\nabla\cdot\left(\bar{\rho}\,\widetilde{\underline{v}''G''}\right) = \nabla\cdot\left(\bar{\rho}D_t\nabla\tilde{G}\right) = \underbrace{-\bar{\rho}D_t|\nabla\tilde{G}|\tilde{\mathcal{K}}}_{\text{CURVATURE}} + \underbrace{\underline{n}\cdot\nabla\left(\bar{\rho}D_t\,\underline{n}\cdot\nabla\tilde{G}\right)}_{\text{DIFFUSION NORMAL TO INTERFACE}}$

NOTICE THAT $S_T^0$ NEEDS MODELLING (SEE, FOR INSTANCE, PAGE 133, PETERS' BOOK)
EITHER A G EQUATION IS SOLVED
AN ALGEBRAIC RELATION BETWEEN $\tilde{\sigma}$ AND $S_T^0$ IS POSED.

⇒ THE RIGHT HAND SIDE OF THE EQUATION FOR $\tilde{G}$ THEN BECOMES:

$-\nabla\cdot\left(\bar{\rho}\,\widetilde{\underline{v}''G''}\right) + \bar{\rho}S_L^0\tilde{\sigma} = -\bar{\rho}D_t|\nabla\tilde{G}|\tilde{\mathcal{K}} + \bar{\rho}S_T^0\tilde{\sigma}$, WHERE $S_T^0$ IS A TURBULENT BURNING VELOCITY GIVEN BY $\bar{\rho}S_T^0\tilde{\sigma} = \bar{\rho}S_L^0\tilde{\sigma} + \underline{n}\cdot\nabla\left(\bar{\rho}D_t\,\underline{n}\cdot\nabla\tilde{G}\right)$

BASED ON A SIMILAR ARGUMENT, $-\nabla\cdot\left(\bar{\rho}\,\widetilde{\underline{v}''G''^2}\right) = \nabla_{||}\cdot\left(\bar{\rho}D_t\nabla_{||}\widetilde{G''^2}\right)$ (↳ TANGENTIAL OPERATOR) ⇒ NO NORMAL TRANSPORT IS INCLUDED FOR G. (↓ NO COUNTER GRADIENT DIFFUSION?)

THE EQUATIONS FOR $\tilde{G}$ AND $\widetilde{G''^2}$ THEN BECOME

$$\begin{cases} \bar{\rho}\dfrac{\partial\tilde{G}}{\partial t} + \bar{\rho}\underline{\tilde{v}}\cdot\nabla\tilde{G} = \bar{\rho}S_T^0\tilde{\sigma} - \bar{\rho}D_t\tilde{\mathcal{K}}\tilde{\sigma} \\ \bar{\rho}\dfrac{\partial\widetilde{G''^2}}{\partial t} + \bar{\rho}\underline{\tilde{v}}\cdot\nabla\widetilde{G''^2} = \nabla_{||}\cdot\left(\bar{\rho}D_t\nabla_{||}\widetilde{G''^2}\right) + 2\bar{\rho}D_t\widetilde{\sigma^2} - c_3\bar{\rho}\dfrac{\varepsilon}{k}\widetilde{G''^2} \end{cases}$$

AN ADDITIONAL TRANSPORT EQUATION FOR $\tilde{\sigma}$ IS NEEDED, WHICH CAN BE WRITTEN AS

$$\bar{\rho}\frac{\partial\tilde{\sigma}_t}{\partial t} + \bar{\rho}\underline{\tilde{v}}\cdot\nabla\tilde{\sigma}_t = \underbrace{-c_0\bar{\rho}\frac{\widetilde{\underline{v}''\underline{v}''}:\nabla\underline{\tilde{v}}}{k}\bar{\sigma}_t}_{\text{STRAINING BY MEAN VELOCITY GRADIENTS}} + \underbrace{c_1\bar{\rho}D_t\frac{(\nabla\tilde{G})^2}{\widetilde{G''^2}}\tilde{\sigma}_t}_{\text{TURBULENT PRODUCTION}} - \underbrace{c_2\bar{\rho}\frac{S_L^0\tilde{\sigma}_t^2}{(\widetilde{G''^2})^{1/2}}}_{\text{KINEMATIC RESTORATION}} - \underbrace{c_3\bar{\rho}\frac{D\tilde{\sigma}_t^3}{\widetilde{G''^2}}}_{\text{SCALAR DISSIPATION}} + \underbrace{\nabla_{||}\cdot\left(\bar{\rho}D_t\nabla_{||}\sigma_t\right)}_{\text{TURBULENT FLUX}}$$

(+ / + / − / − / +/−)

WITH $\tilde{\sigma} = 1 + \tilde{\sigma}_t$ (SEE PETERS 1999, JFM FOR DERIVATION).

AS NOTICED BEFORE, THE FLAMELET EQUATIONS ARE SOLVED IN THE NORMAL COORDINATE $Y_n = \frac{G-G_0}{\sigma}$.

THEN, THE FAVRE MEAN OF A SCALAR $Y_i$ IS GIVEN BY

$$\tilde{Y}_i = \int_{-\infty}^{+\infty}\int_0^{+\infty} Y_i\left(\frac{G-G_0}{\sigma}, t\right)\delta\left(\sigma - \langle\sigma|_{G=G_0}\rangle\right)\tilde{P}(G;\underline{x},t)\,d\sigma\,dG =$$

(STEADY FLAMELETS)

$$= \int_{-\infty}^{+\infty} Y_i\left(\frac{G-G_0}{\langle\sigma|_{G=G_0}\rangle}, t\right)\tilde{P}(G;\underline{x},t)\,dG, \quad \text{WITH} \quad \tilde{P}(G,\underline{x},t) = \frac{1}{\sqrt{2\pi\left(\widetilde{G''^2}\right)_0}}\,e^{-\frac{(G-\tilde{G})^2}{2\left(\widetilde{G''^2}\right)_0}}$$

($\langle\sigma|_{G=G_0}\rangle \equiv \tilde{\sigma}|_{G=G_0}$; THE PRESUMED PDF.)

## ARTIFICIALLY-THICKENED FLAMES

AN INEXPENSIVE SOLUTION, OF PARTICULAR INTEREST FOR LES OF PREMIXED TURBULENT COMBUSTION, CONSISTS ON MULTIPLYING THE DIFFUSION COEFFICIENTS BY A FACTOR $F > 1$ AND DIVIDING THE REACTION TERMS BY A FACTOR $F > 1$. IN THIS WAY, AND ACCORDING TO SINGLE-STEP LARGE-ACTIVATION-ENERGY SCALINGS IN LAMINAR PLANAR PREMIXED FLAMES, THE PROPAGATION SPEED $S_L^0 \sim (D/t_F)^{1/2}$ REMAINS THE SAME BUT THE FLAME THICKNESS $\delta_L^0$ IS MULTIPLIED BY F. THEN, IF $\Delta < F\delta_L^0$, WITH $\Delta$ THE FILTER SCALE, THE THICKENED FRONT CAN BE RESOLVED IN LES. NOTICE HOWEVER THAT, SINCE THE CHEMICAL TIME IS ARTIFICIALLY CHANGED IN THIS PROCEDURE, THE INTERACTION OF TURBULENCE WITH THE FLAME IS CHANGED (BY FOR INSTANCE, CHANGING Da, $Re_t$ AND Ka IN THE COMBUSTION DIAGRAM ($Re_t$ IS DECREASED, Da IS DECREASED, Ka IS INCREASED BY A FACTOR F), IN PRACTICE, THICKENING IS NOT ACTIVATED EVERYWHERE (MIXING WOULD OTHERWISE BE AFFECTED) BUT A SENSOR THAT LOCATES ZONES WITH NON-ZERO CHEMICAL-REACTION TERMS ACTIVATES THE THICKENING FACTOR F.

# PREMIXED BURNERS

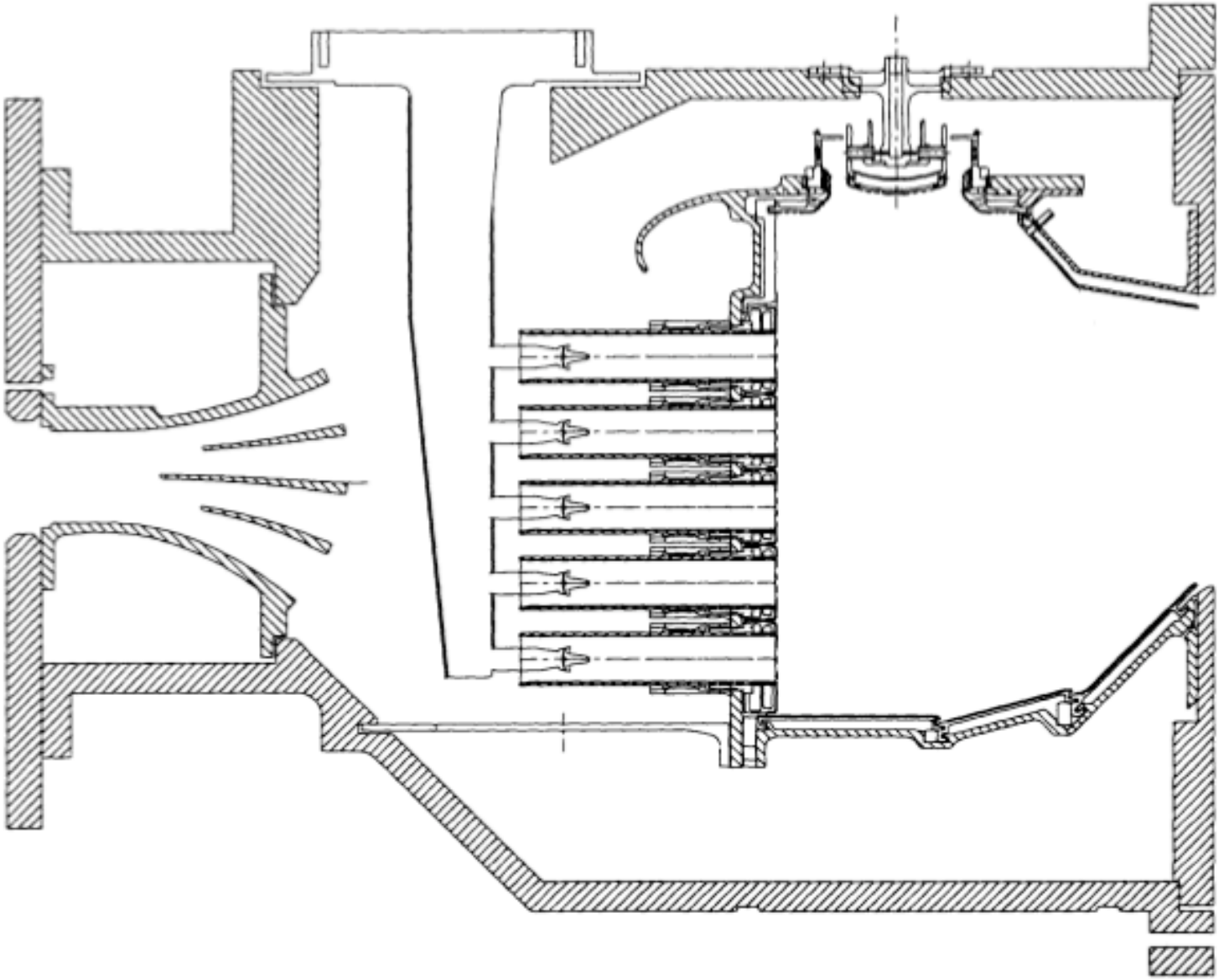
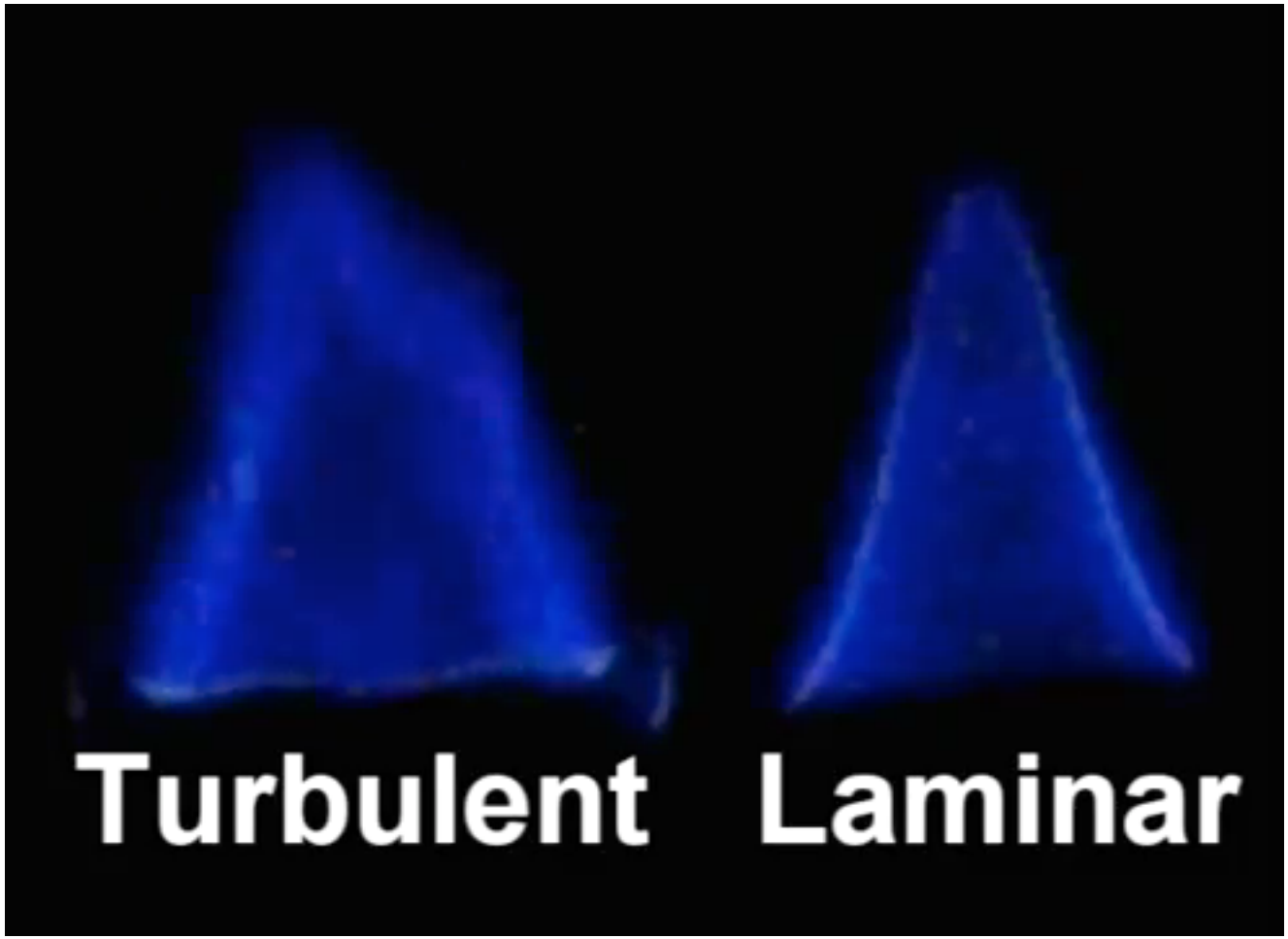
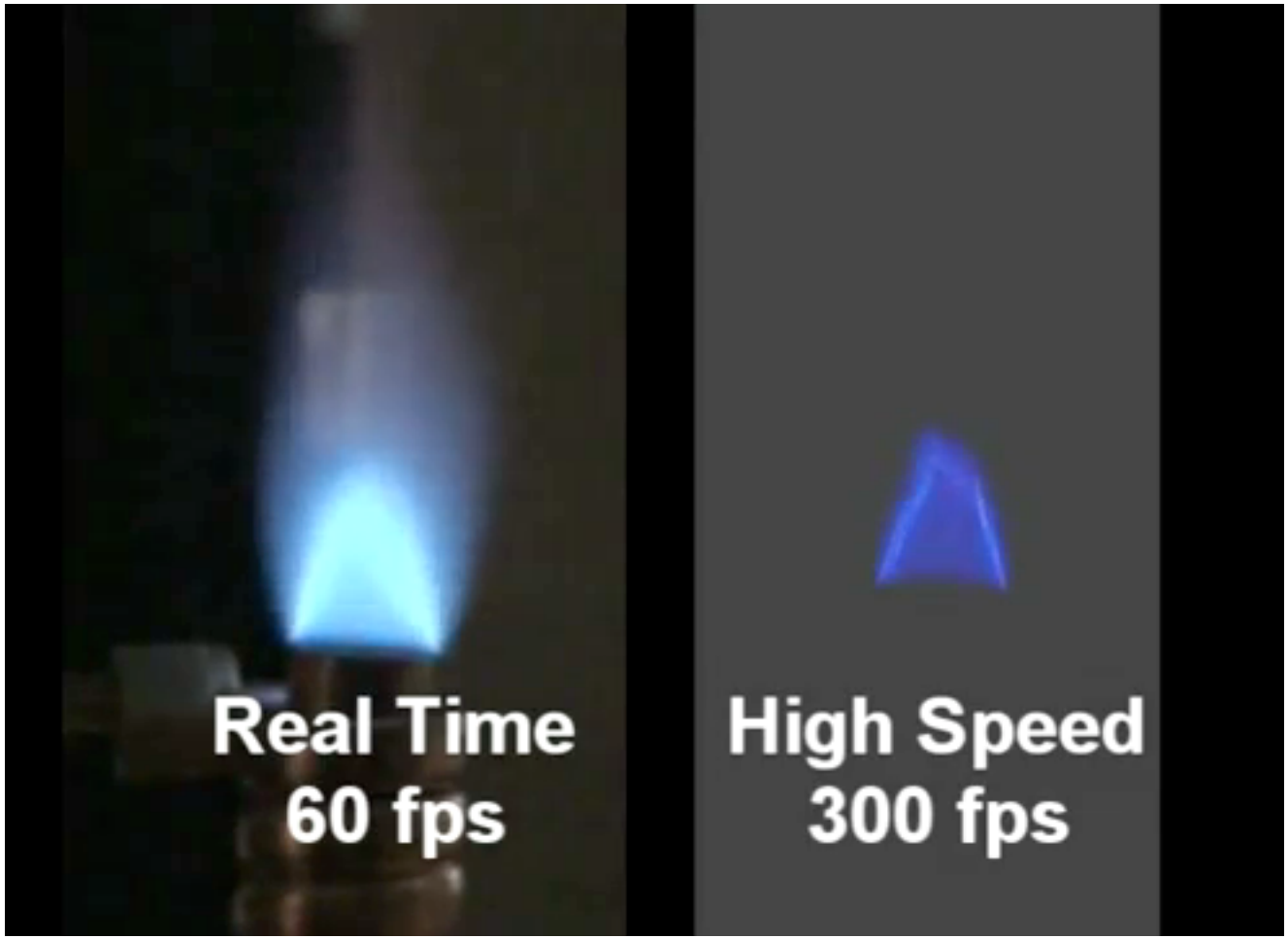


**Figure 11. LPP MRA Combustor Concept 5**

# PREMIXED BURNERS



# PREMIXED BURNERS



CLANET+SEARBY (1998)

DARRIEUS-LANDAU INSTABILITY

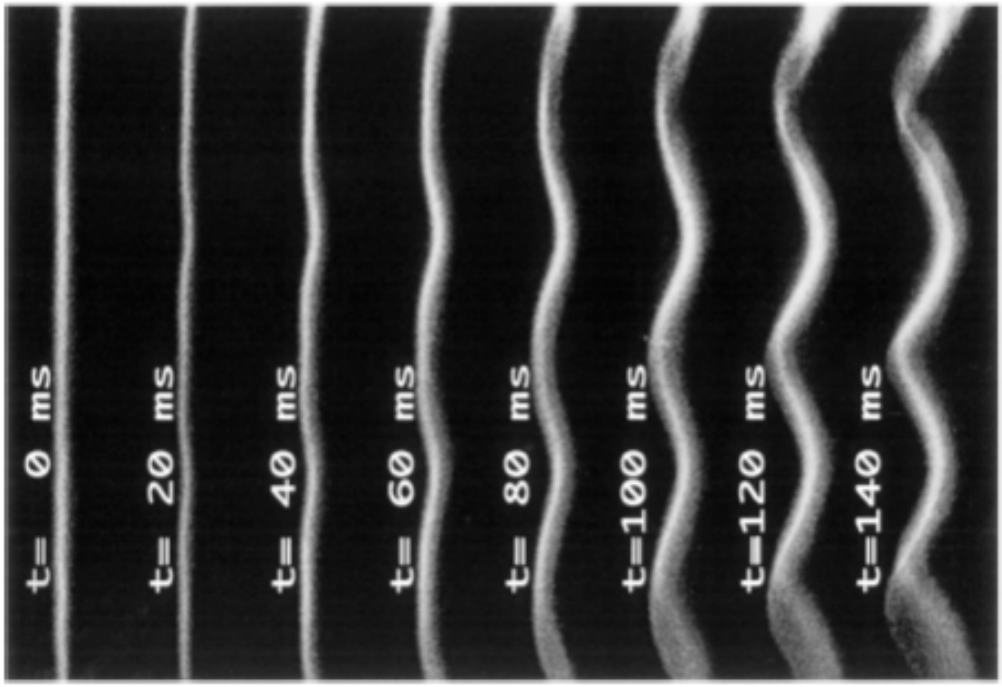
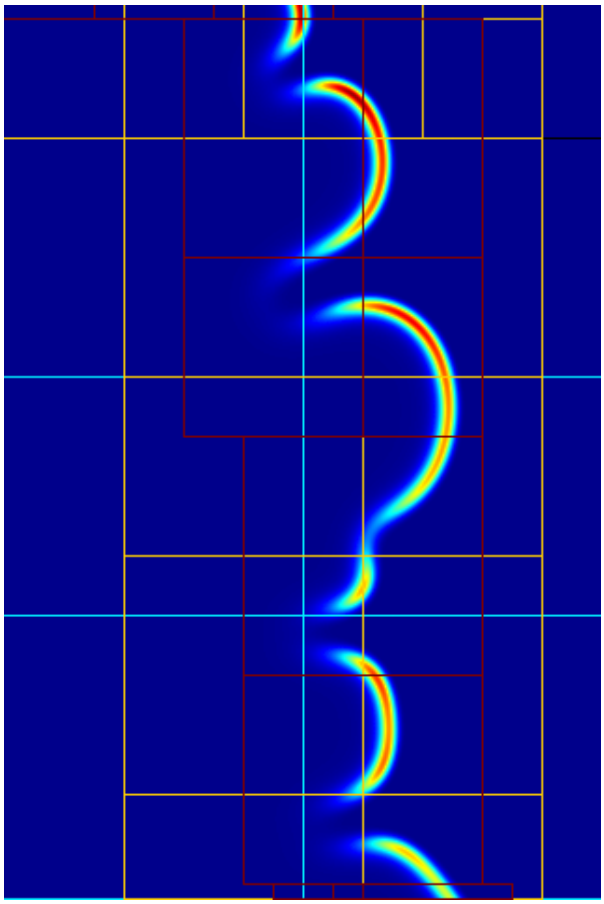


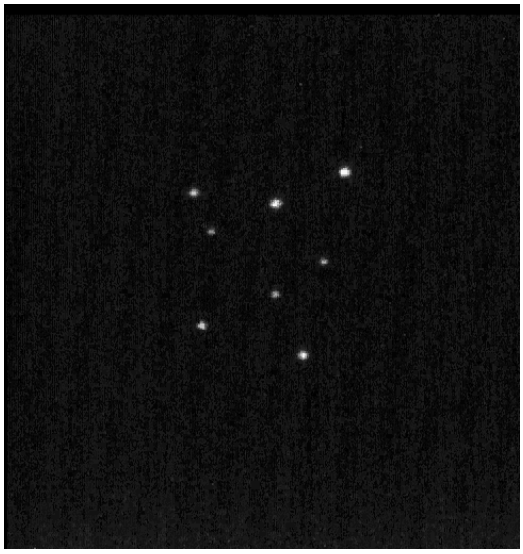

FIG. 6. Images taken from high speed film of growth of instability. Framing rate 500 images/s, wavelength 2 cm, flame speed 11.5 cm/s.

# Cellular Flames

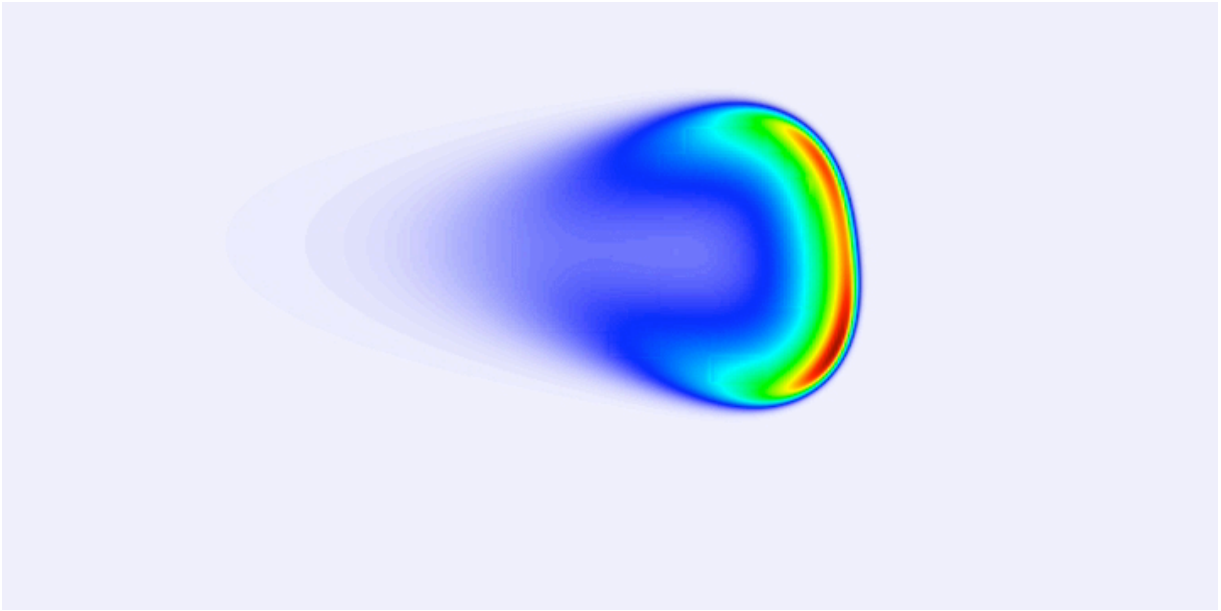


CELLULAR FLAMES H2/O2

RONNEY



FLAME BALLS



CELLULAR FLAMES H2/O2

GRCAR (2008)

FIG 4

FOR $Le \neq 1$, CURVATURE IS ALSO IMPORTANT.

IF THIS CONFIGURATION IS USED, ONLY STRAIN IS ACCOUNTED FOR IN $\mathcal{K}$

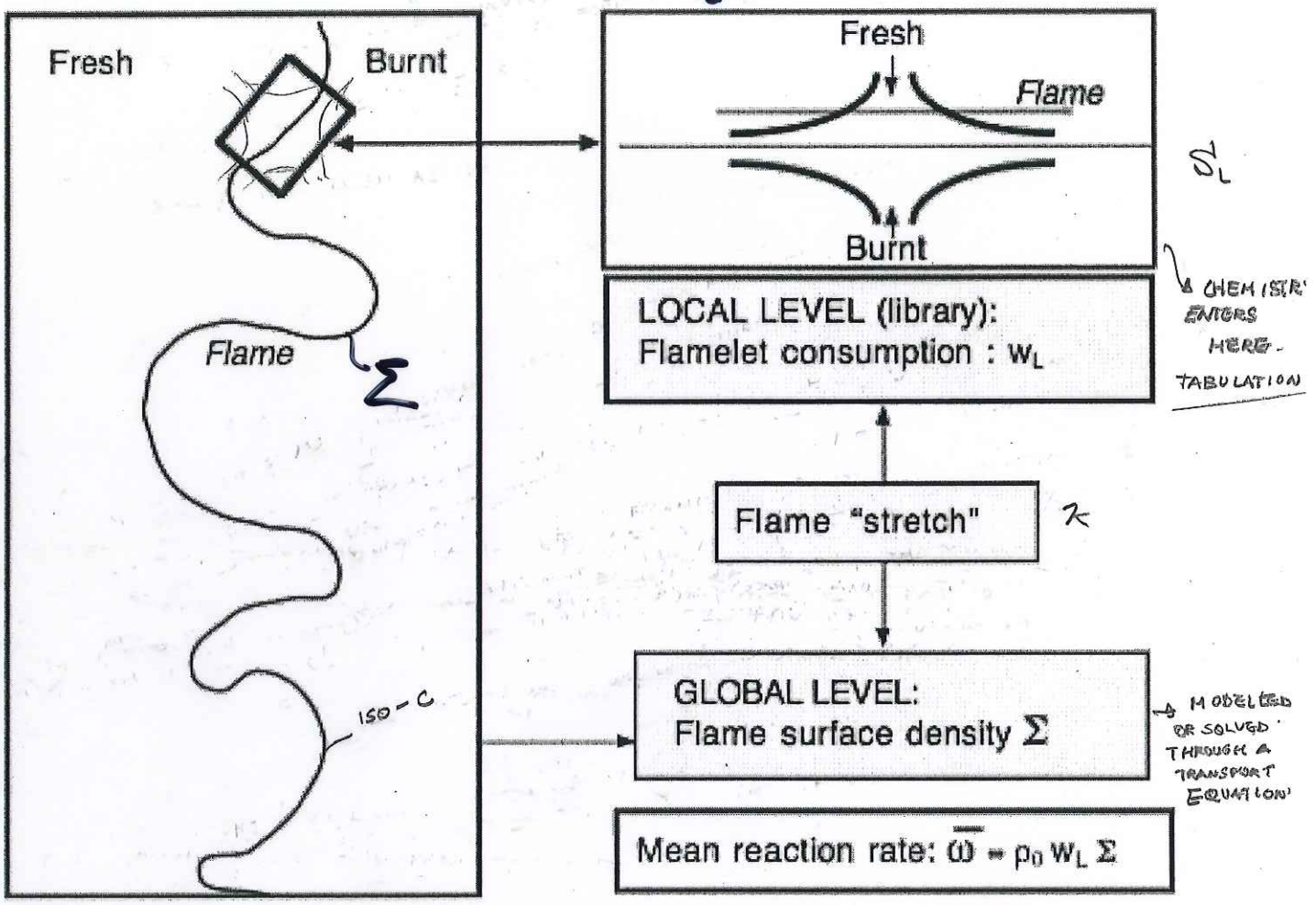



Figure 5.30: Flame surface density concepts for turbulent premixed flames.

CURVATURE EFFECTS TEND TO CANCEL OUT WHEN THE MEAN FLAMELET SPEED (AVERAGED ALONG THE FLAME FRONT) IS COMPUTED. BUT STRAIN EFFECTS PERSIST (HAWORTH + POINSOT, 1992)

POINSOT + VEYNANTE (2005)

HAWORTH + POINSOT (1992)

FIG 5

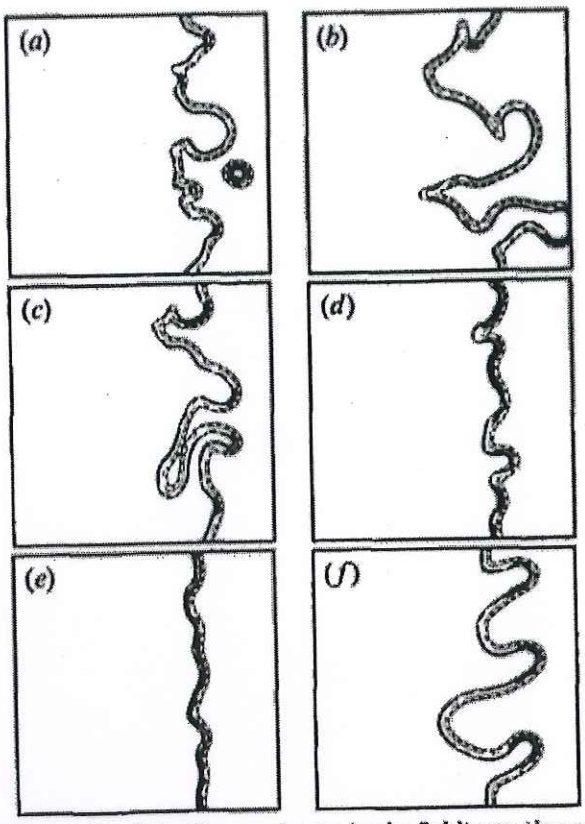
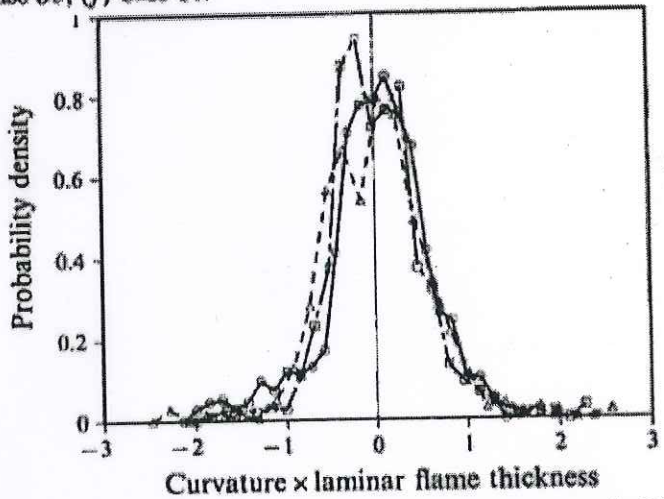
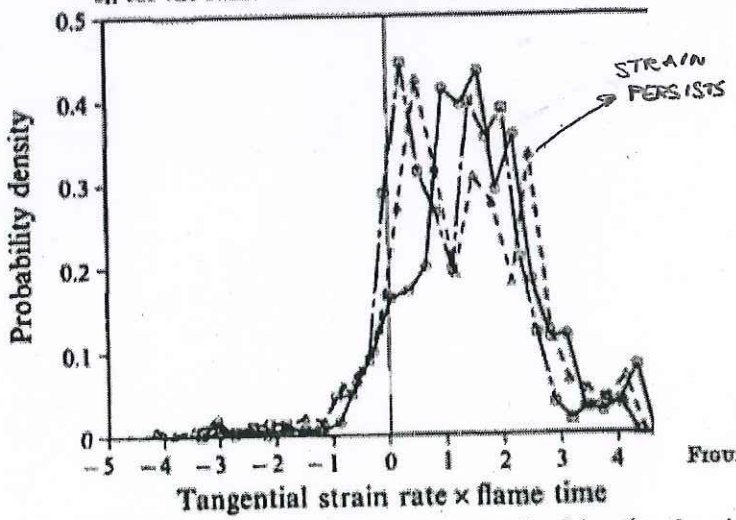



FIGURE 4. Examples of normalized (by the maximum in the field) reaction rate contours for several flames. Isocontours 0.015, 0.05, 0.25, and 0.6 are plotted: (*a*) Case 4*b*; (*b*) Case 4*d*; (*c*) Case 3*b*; (*d*) Case 6*c*; (*e*) Case 5*c*; (*f*) Case 8*c*.

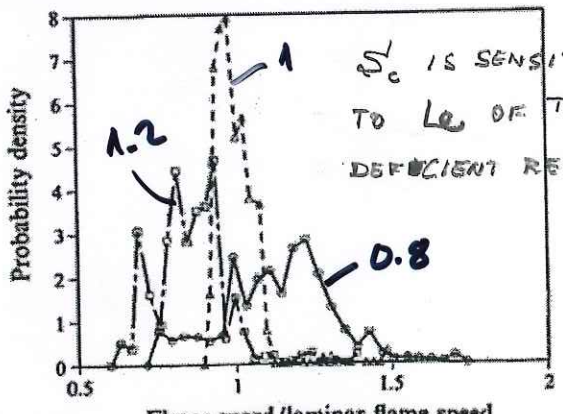



OVERALL CURVATURE EFFECT TEND TO CANCEL

FIGURE 6. P.d.f.s of flame curvature $\mathscr{R}^{-1}$ normalized by the undisturbed laminar flame thickness $\delta_u$ for the same Lewis number: ○, Case 1*b*, $Le = 0.8$; △, Case 2*b*, $Le = 1.0$; □, Case 3*b*, $Le = 1.2$.




STRAIN PERSISTS




1

1.2

0.8

$S_c$ IS SENSITIVE TO $Le$ OF THE DEFICIENT REACTAI

FIGURE 12. P.d.f.s of normalized local flamelet speed $s_l^*$: ○, Case 1*b*, $Le$ △, Case 2*b*, $Le = 1.0$; □, Case 3*b*, $Le = 1.2$.

FIGURE 7. P.d.f.s of flame tangential strain rate $a_t$ normalized by the chemical time $\tau_l$ for the same Lewis number: ○, Case 1*b*, $Le = 0.8$; △, Case 2*b*, $Le = 1.0$; □, Case 3*b*, $Le = 1.2$

FIG 3 BML MODEL

VEYNANTE + POINSOT (2005)

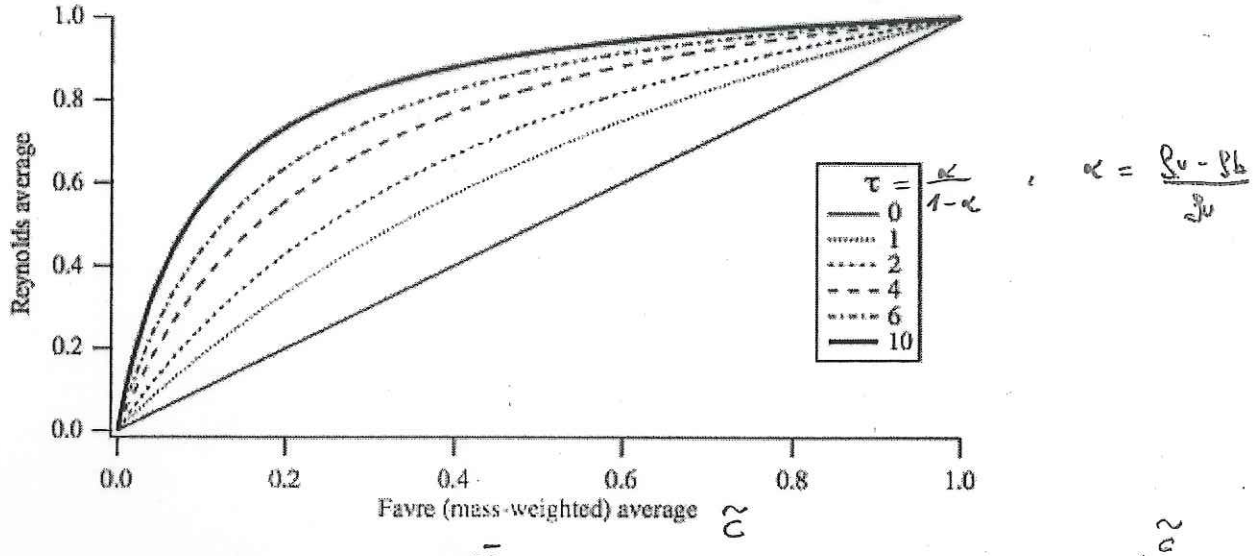



**Figure 5.8:** Reynolds average temperature $\overline{\Theta}$ as a function of the Favre average temperature $\widetilde{\Theta}$ for various values of the heat release factor $\tau$, assuming a bimodal distribution ($\Theta = 0$ or $\Theta = 1$) of the reduced temperature $\Theta$ (Eq. 5.15).

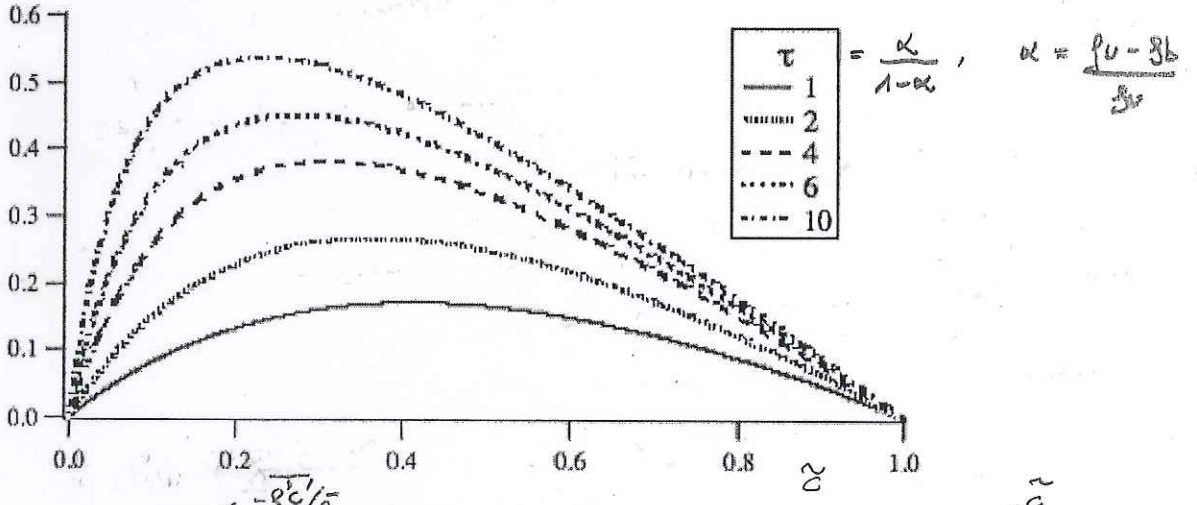



**Figure 5.9:** Correlation $-\overline{\rho' \Theta'}/\overline{\rho}$ as a function of the Favre averaged progress variable $\widetilde{\Theta}$ for various values of the heat release factor $\tau$, assuming a bimodal distribution ($\Theta = 0$ or $\Theta = 1$) of the reduced temperature $\Theta$ (Eq. 5.16).

# DNS

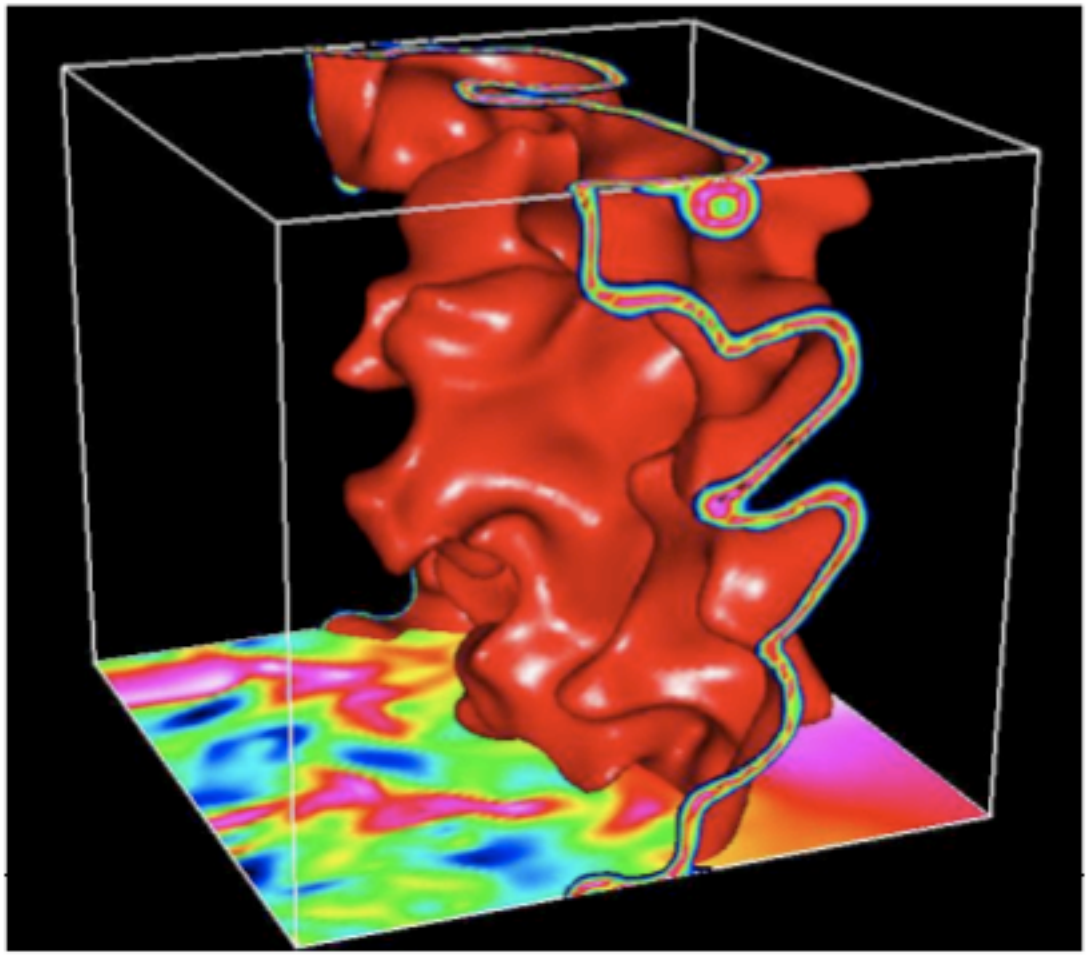


**Figure 4.8:** DNS of a premixed flame interacting with three-dimensional isotropic turbulence (Boger et al.[47]). An isosurface of temperature is visualized. The reaction rate is presented in two planes which are normal to the mean flame front. The vorticity field, corresponding to turbulent motions, is also displayed in the bottom plane.

# Cellular Flames

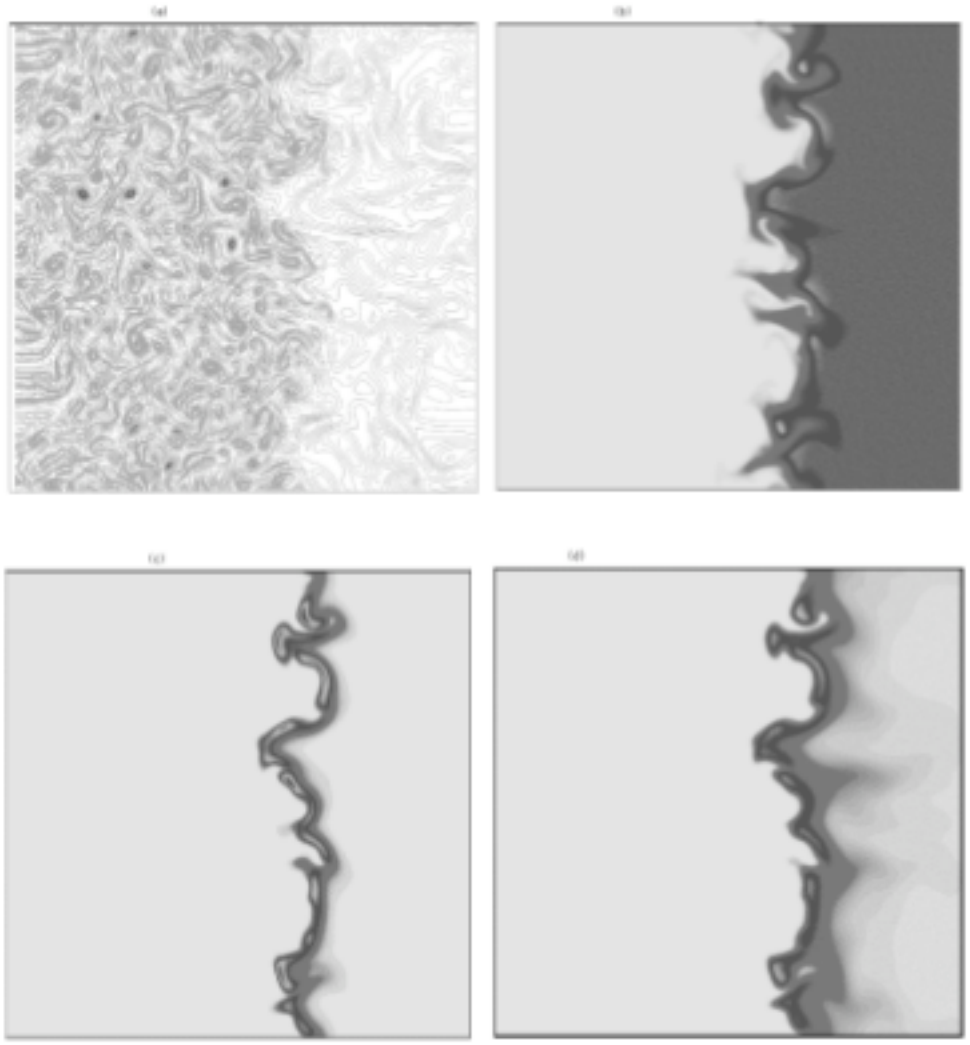


**Figure 5.58**: DNS of a turbulent $H_2/O_2$ flame with the 9-species/19-reactions Miller scheme (Baum et al.[28] reprinted with permission by Cambridge University Press): vorticity (a), temperature (b), heat release (c) and OH mass fraction (d) fields.

FIG 6

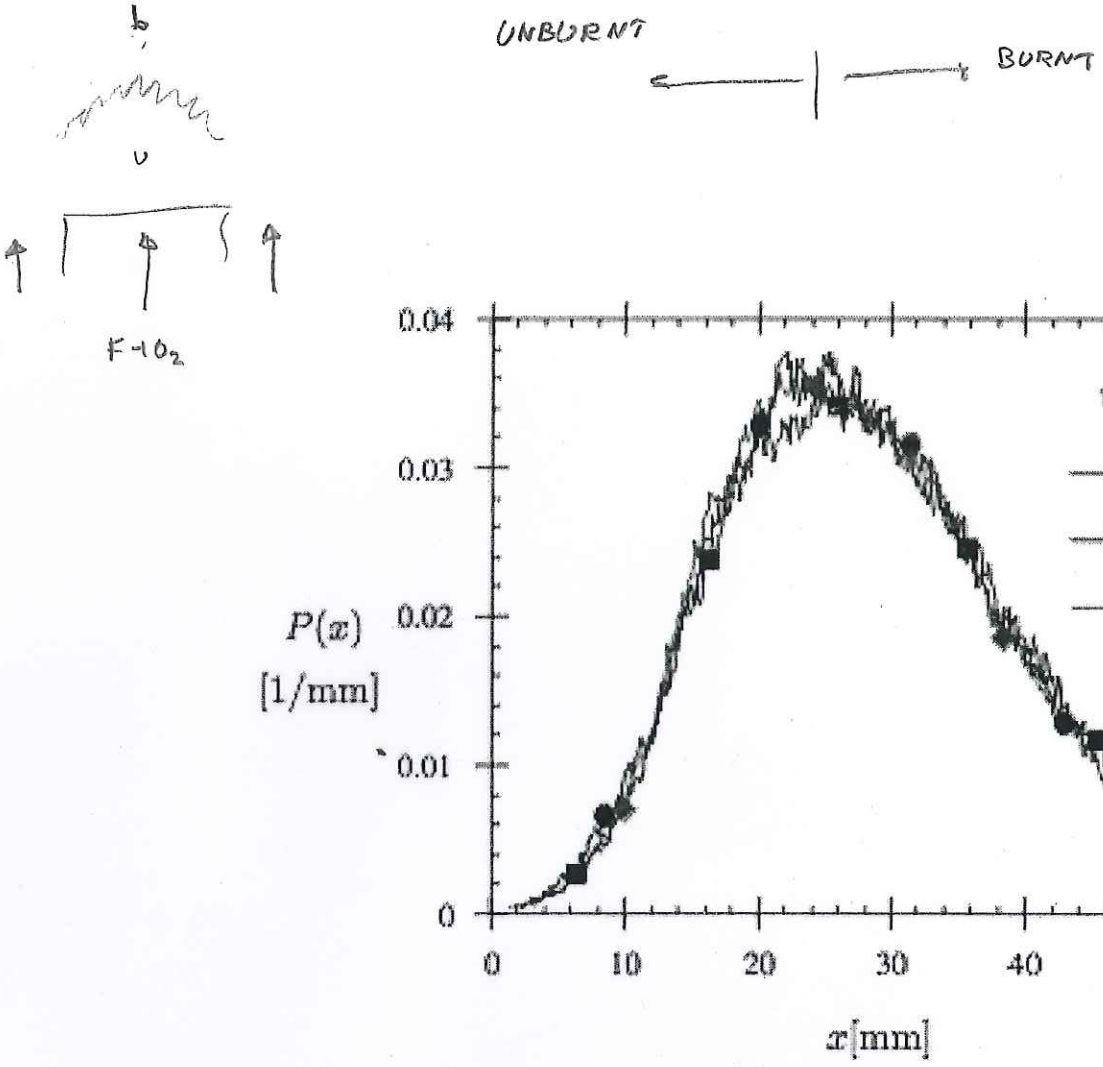
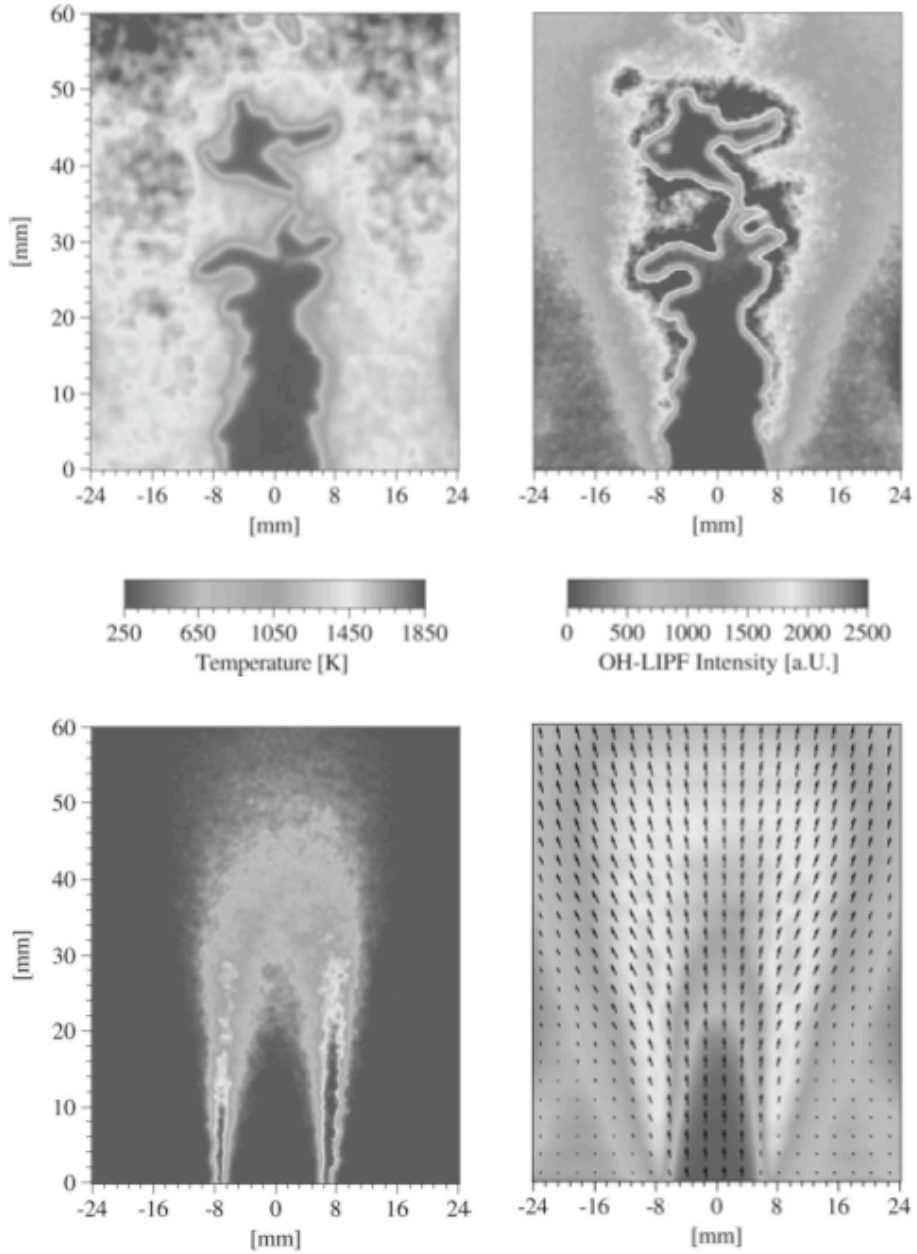
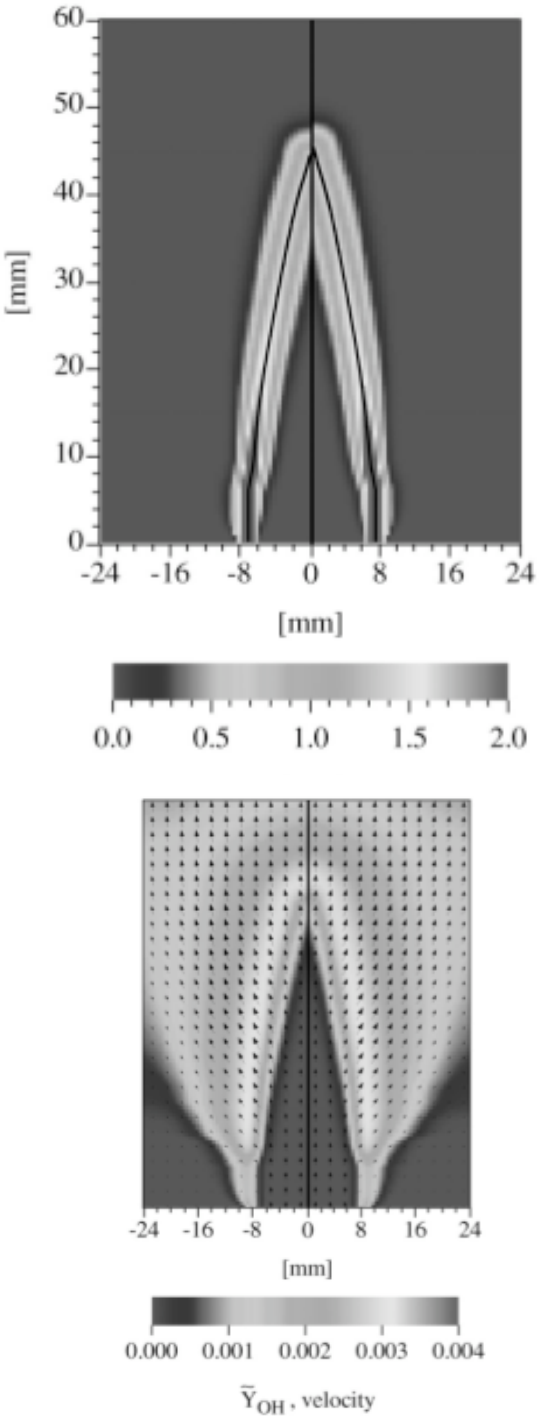



**Figure 2.19.** The probability density of finding the instantaneous flame front at the axial position $x$ in a turbulent flame stabilized on a weak swirl burner (cf. Figure 2.7). Measurements by Plessing et al. (2000). (Reprinted with permission by The Combustion Institute.)

# Level Set

RANS (Peters, 2000)



# Level Set

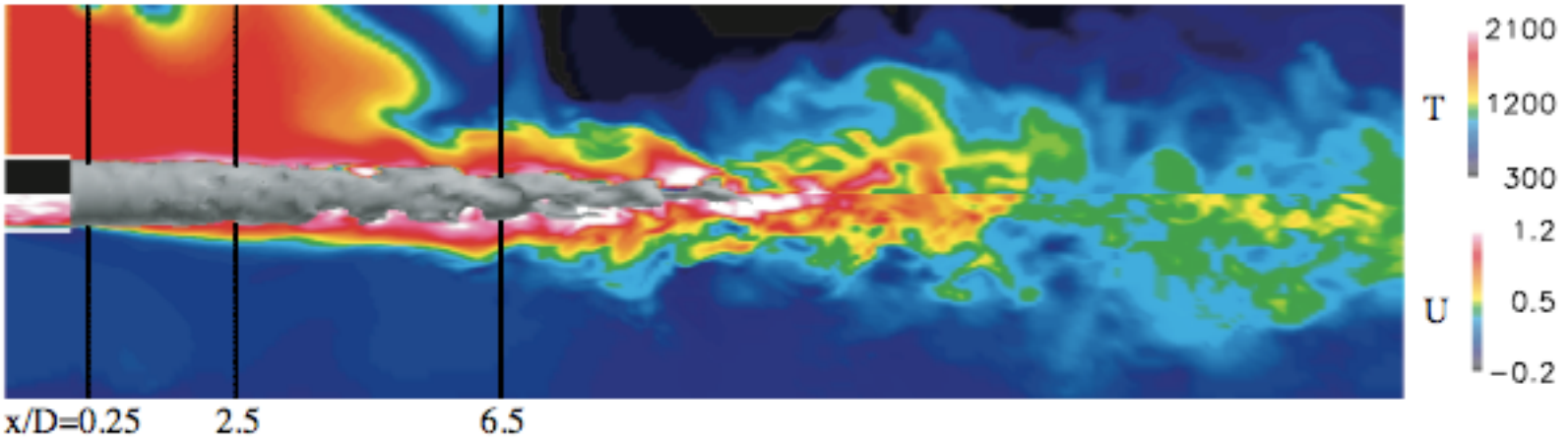



Fig. 2. Instantaneous flame position (gray surface), temperature distribution (top part), and axial velocity distribution (bottom part)

LES (Pitsch & Duchamp, 2002)

# Thickened flames

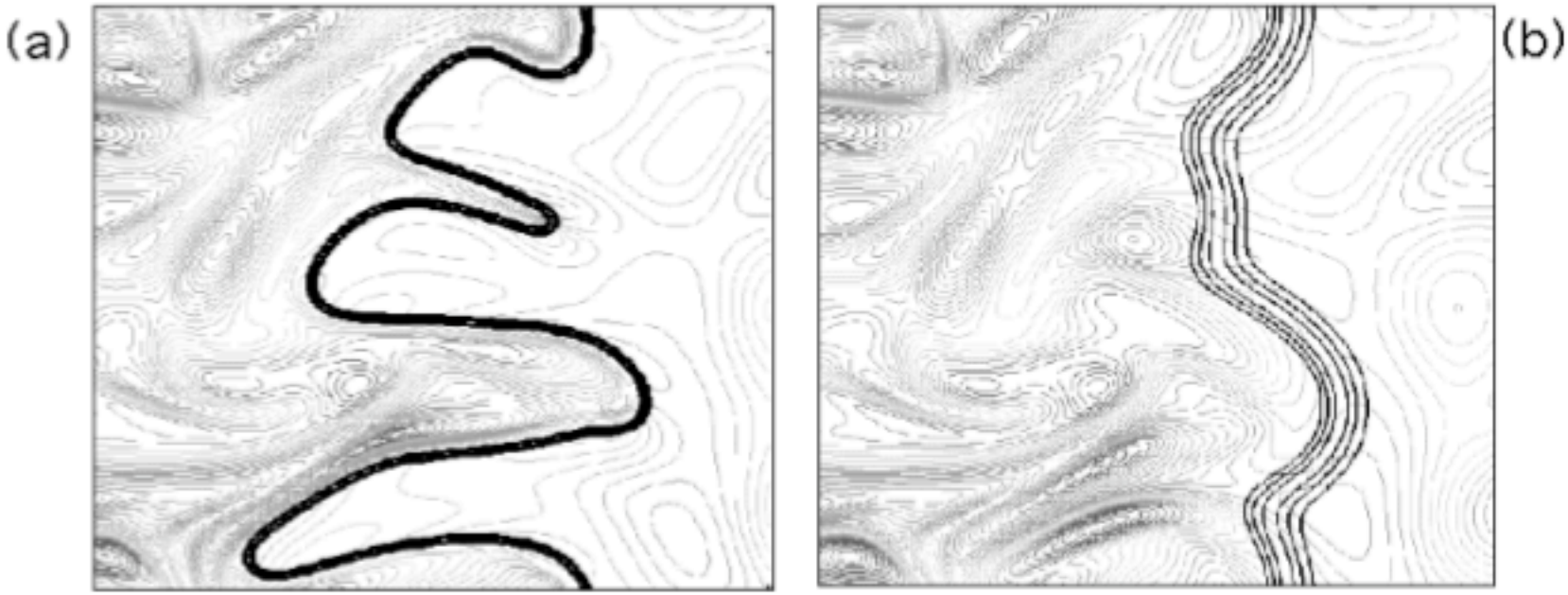



**Figure 5.44:** DNS of flame turbulence interactions. Reaction rate and vorticity fields are superimposed. (a) reference flame; (b) flame artificially thickened by a factor $F = 5$. Because of the change in the length scale ratio $l_t / {}^{0}_{L}$, combustion/turbulence interaction is changed and the thickened flame is less wrinkled by turbulence motions. This effect can be parametrized using a subgrid scale model.

(Poinsot & Veynante, 2005)

STANFORD MECHANICAL ENGINEERING

**ME 471: TURBULENT COMBUSTION**

**Spring 2012**

# PART III:

# Turbulent Non-premixed Combustion

J. Urzay

# NON-PREMIXED TURBULENT COMBUSTION

## THE MIXTURE-FRACTION VARIABLE

CONSIDER THE SINGLE CHEMICAL REACTION $F + bO_2 \longrightarrow P$. IF $F = C_m H_m$, THEN $b = m + \frac{m}{4}$ FOR COMPLETE COMBUSTION $\left(P = m CO_2 + \frac{m}{2} H_2O\right)$. THEN, THE CONSERVATION EQUATIONS FOR THE SPECIES (FUEL AND OXIDIZER) ARE:

$$\rho \frac{\partial Y_F}{\partial t} + \rho \underline{v} \cdot \nabla Y_F = \nabla \cdot (\rho D_F \nabla Y_F) + \dot{w}_F$$
$$\rho \frac{\partial Y_{O_2}}{\partial t} + \rho \underline{v} \cdot \nabla Y_{O_2} = \nabla \cdot (\rho D_{O_2} \nabla Y_{O_2}) + \dot{w}_{O_2}$$

NOTE THAT $\dot{w}_F = -W_F \dot{\omega}$ AND $\dot{w}_{O_2} = -b W_{O_2} \dot{\omega}$ WHERE $\dot{\omega}$ IS THE RATE OF REACTION.

DEFINING $s = \frac{b W_{O_2}}{W_F}$ THE OXIDIZER MASS REACTING WITH THE UNIT MASS OF FUEL IN STOICHIOMETRIC PROPORTIONS ($s = 8$ FOR $H_2/O_2$, $s = 4$ FOR $CH_4/O_2$), THEN THE SPECIES EQUATIONS BECOME

$$\rho \frac{\partial Y_F}{\partial t} + \rho \underline{v} \cdot \nabla Y_F = \nabla \cdot (\rho D_F \nabla Y_F) + W_F \dot{\omega}$$
$$\rho \frac{\partial Y_{O_2}}{\partial t} + \rho \underline{v} \cdot \nabla Y_{O_2} = \nabla \cdot (\rho D_{O_2} \nabla Y_{O_2}) - s W_F \dot{\omega}$$

IF $D_F = D_{O_2} = D$, THESE TWO TRANSPORT EQUATIONS CAN BE COMBINED (EXACTLY) TO GIVE A SINGLE TRANSPORT EQUATION FOR $Z$, WITH

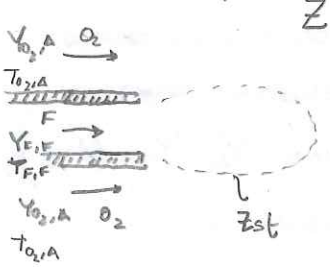
$$\rho \frac{\partial Z}{\partial t} + \rho \underline{v} \cdot \nabla Z = \nabla \cdot (\rho D \nabla Z) \qquad (1)$$

WHERE $Z$ IS A CONSERVED SCALAR (A SCALAR NOT INFLUENCED DIRECTLY BY THE CHEMICAL REACTION) GIVEN BY

$$Z = \frac{s Y_F - Y_{O_2} + Y_{O_2,A}}{s Y_{F,F} + Y_{O_2,A}} = \frac{s \hat{Y}_F - \hat{Y}_{O_2} + 1}{s + 1} \qquad (2)$$

$Z = 0$ IN THE AIR STREAM ($Y_{O_2} = Y_{O_2,A}$, $Y_F = 0$)

$Z = 1$ IN THE FUEL STREAM ($Y_F = Y_{F,F}$, $Y_{O_2} = 0$)




WITH $\hat{Y}_F = Y_F / Y_{F,F}$ AND $\hat{Y}_{O_2} = Y_{O_2} / Y_{O_2,A}$, AND $s = s \frac{Y_{F,F}}{Y_{O_2,A}}$ TYPICALLY A LARGE NUMBER IN COMBUSTION APPLICATIONS IN AIR ($s \approx 33$ IN $H_2$/AIR, $s \approx 18$ IN $CH_4$/AIR)

IN THIS CONTEXT, $Z$ IS A COUPLING FUNCTION OR SHVAB-ZEL'DOVICH VARIABLE. A QUANTITY CALLED STOICHIOMETRIC MIXTURE FRACTION IS DEFINED AS $Z_{st} = \frac{1}{1+s}$, OR EQUIVALENTLY, AS THE MIXTURE FRACTION $Z$ EVALUATED IN STOICHIOMETRIC PROPORTIONS $\left(Y_F / Y_{O_2} \to 1/s\right)$. IN GENERAL, $Z_{st}$ IS A SMALL NUMBER ($Z_{st} \sim 0.029$ FOR $H_2$/AIR, $Z_{st} \sim 0.053$ FOR $CH_4$/AIR), WHICH INDICATES THAT STOICHIOMETRIC CONDITIONS ARE TYPICALLY ATTAINED FAR WITHIN THE AIR SIDE.

THIS LIMIT CAN INVOLVE $Y_F, Y_{O_2} \to 0$ SIMULTANEOUSLY

THE ENTHALPY EQUATION CAN BE WRITTEN AS $\rho \frac{\partial T}{\partial t} + \rho \underline{v} \cdot \nabla T = \nabla \cdot \left(\frac{\lambda}{c_p} \nabla T\right) + \frac{\dot{w}_T}{c_p}$, WHERE $c_p$ HAS BEEN ASSUMED TO BE CONSTANT AND $\dot{w}_T = -\sum h_i^\circ \dot{w}_i = (h_F^\circ W_F - h_P^\circ W_P)\dot{\omega} = q s W_F \dot{\omega}$, WITH $q$ THE CHEMICAL HEAT RELEASED PER UNIT MASS OF FUEL. ADDITIONAL CONSERVED SCALARS COULD BE OBTAINED BY COMBINING THE SPECIES AND ENTHALPY EQUATION IN THE FOLLOWING MANNER IF $Le = \frac{D}{D_T} = 1$:

$$\rho \frac{\partial Y_F}{\partial t} + \rho \underline{v} \cdot \nabla Y_F = \nabla \cdot (\rho D \nabla Y_F) - W_F \dot{\omega}$$
$$\rho \frac{\partial T}{\partial t} + \rho \underline{v} \cdot \nabla T = \nabla \cdot (\rho D_T \nabla T) + \frac{q s W_F \dot{\omega}}{c_p}$$

$$\varphi_F = s Y_F + \frac{c_p}{q}(T - T_{O_2,A})$$

WITH $\rho \frac{\partial \varphi_F}{\partial t} + \rho \underline{v} \cdot \nabla \varphi_F = \nabla \cdot (\rho D \nabla \varphi_F)$

SUBJECT TO $\varphi_F = 0$ $(Z = 0)$ AND $\varphi_{F_s} = s Y_{F,F} + \frac{c_p}{q}(T_{F,F} - T_{O_2,A})$ AT $Z = 1$.

$\Rightarrow \varphi_F = \varphi_{F_s} Z$ IS A SOLUTION (*)

AND $\rho\frac{\partial Y_{O_2}}{\partial t} + \rho \underline{v}\cdot\nabla Y_{O_2} = \nabla\cdot(\rho D \nabla Y_{O_2}) - s W_F \dot{\omega}$

$\rho\frac{\partial T}{\partial t} + \rho \underline{v}\cdot\nabla T = \nabla\cdot(\rho D_T \nabla T) + \frac{q s W_F}{c_p}\dot{\omega}$

$\Rightarrow$ $\varphi_{O_2} = Z\,\varphi_{O_2 S}$ IS A SOLUTION (**)

$\varphi_{O_2} = Y_{O_2} + \frac{c_p}{q}(T - T_{O_2,A}) - Y_{O_2,A}$

WITH $\rho\frac{\partial \varphi_{O_2}}{\partial t} + \rho \underline{v}\cdot\nabla \varphi_{O_2} = \nabla\cdot(\rho D \nabla \varphi_{O_2})$

AND $\varphi_{O_2} = 0$ AT $Z = 0$, $\varphi_{O_{2S}} = \frac{c_p}{q}(T_{F,F} - T_{O_2,A}) - Y_{O_2,A}$ AT $Z = 1$

FROM (*) AND (**) THE EXPRESSIONS

$$Y_F = Y_{F,F} Z + \frac{c_p}{q s}\left[(T_{F,F} - T_{O_2,A})Z - (T - T_{O_2,A})\right] \quad (3)$$

$$Y_{O_2} = Y_{O_2,A}(1 - Z) + \frac{c_p}{q}\left[(T_{F,F} - T_{O_2,A})Z - (T - T_{O_2,A})\right] \quad (4)$$

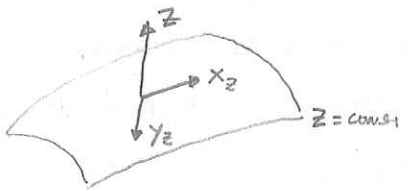
ARE OBTAINED. WITH THESE EXPRESSIONS, THE INITIAL 3-PDE PROBLEM IS REDUCED TO INTEGRATING

$$\rho\frac{\partial Z}{\partial t} + \rho \underline{v}\cdot\nabla Z = \nabla\cdot(\rho D \nabla Z)$$

$$\rho\frac{\partial T}{\partial t} + \rho \underline{v}\cdot\nabla T = \nabla\cdot(\rho D \nabla T) - \frac{q s W_F}{c_p}\dot{\omega}$$

WITH $Y_F = Y_F(Z,T)$ AND $Y_{O_2} = Y_{O_2}(Z,T)$ GIVEN BY (3) AND (4)

IF $\rho D$ IS INDEPENDENT OF $T$ AND IF TEMPERATURE VARIATIONS HAVE NEGLIGIBLE EFFECTS ON THE FLUID DYNAMICS, THE EQUATION FOR $Z$ CAN BE INTEGRATED INDEPENDENTLY TO OBTAIN A SOLUTION $Z = Z(\underline{x}, t)$, WHICH REDUCES THE PROBLEM TO INTEGRATING THE ENERGY EQUATION. IN ABSENCE OF COMBUSTION, THESE EQUATIONS REDUCE TO $Y_F = Y_{F,F} Z$ AND $Y_{O_2} = Y_{O_2,A}(1 - Z)$, WITH $T = T_{O_2,A} + Z(T_{F,F} - T_{O_2,A})$ THE FROZEN TEMPERATURE. NOTICE HOWEVER THAT EXPRESSIONS (3) AND (4) ARE ONLY <u>EXACT</u> WHEN i) $D_F = D_{O_2} = D$, ii) $D_T = D$ $(Le = 1)$, iii) THE CHEMICAL REACTION IS A SINGLE STEP, AND iv) THE CONDITIONS $Y_{F,F}$, $T_{F,F}$, $Y_{O_2,A}$ AND $T_{O_2,A}$ ARE HOMOGENEOUS AT THE BOUNDARIES. IN THE MOST GENERAL CASE IN WHICH THE BOUNDARY TEMPERATURE, FOR INSTANCE, $T_{F,F}$, VARIES WITH POSITION AT THE FUEL INLET $(Z = 1)$, THEN VARIATIONS OF TEMPERATURE ALONG $Z = $ CONST ISO SURFACES WOULD BE INDUCED. IN THAT CASE, (*) AND (**) WOULD NOT HOLD SINCE $\varphi_{O_2 S}$ AND $\varphi_{F,S}$ WOULD NOT BE CONSTANTS AND $\mathcal{L}(Z\varphi_{O_2 S}) \neq 0$ / $\mathcal{L}(Z\varphi_{F,S}) \neq 0$ WITH $\mathcal{L} = \rho\frac{\partial}{\partial t} + \rho \underline{v}\cdot\nabla - \nabla\cdot(\rho D \nabla)$. NOTE THAT, IN THE MOST GENERAL CASE, A CHANGE OF VARIABLES $(x, y, z) \to (x_z, y_z, Z)$, WITH $x_z$ AND $y_z$ DISTANCES ALONG SURFACES OF CONSTANT $Z$, LEADS TO




$$\rho\frac{\partial \phi}{\partial t} + \rho \underline{v}_\perp\cdot\nabla_\perp\phi = \dot{w}_\phi + \chi\frac{\partial^2\phi}{\partial Z^2} + \nabla_\perp\cdot(\rho D \nabla_\perp\phi) + Z\rho D \nabla Z\cdot\frac{\partial}{\partial Z}(\nabla_\perp\phi) + \nabla Z\cdot\nabla_\perp\phi\frac{\partial}{\partial Z}(\rho D), \quad (5)$$

$\phi = Y_F$, $Y_{O_2}$, OR $T$.

WHERE THE CHANGES $\nabla = \nabla_\perp + \nabla Z\frac{\partial}{\partial Z}$, $\frac{\partial}{\partial t} = \frac{\partial Z}{\partial t}\cdot\frac{\partial \phi}{\partial Z} + \frac{\partial}{\partial t}$ HAVE BEEN USED. IN THIS FORMULATION, $\chi = D|\nabla Z|^2$ IS A SCALAR DISSIPATION RATE, WHICH IS A MEASURE OF A DIFFUSION TIME THROUGH THE STOICHIOMETRIC SURFACE.

NOTICE THAT WHEN THE IN-PLANE GRADIENTS OF $\phi$ DISSAPEAR, THEN (5) REDUCES TO

$$\rho\chi\frac{\partial^2\phi}{\partial Z^2} = -\dot{w}_\phi \quad \text{FOR STEADY CONDITIONS.} \qquad \begin{cases} \rho\chi\dfrac{\partial^2 T}{\partial Z^2} = \dfrac{\dot{w}_T}{c_p}, \quad \rho\chi\dfrac{\partial^2 Y_{O_2}}{\partial Z^2} = -\dot{w}_{O_2} \\ \rho\chi\dfrac{\partial^2 Y_F}{\partial Z^2} = -\dot{w}_F \end{cases} \qquad (6)$$

WHEN CHEMICAL REACTIONS ARE FROZEN, $\chi\dfrac{\partial^2 Y_F}{\partial Z^2} = \chi\dfrac{\partial^2 Y_{O_2}}{\partial Z^2} = \chi\dfrac{\partial^2 T}{\partial Z^2} = 0$ AND THE PROFILES OF $Y_F$, $Y_{O_2}$ AND $T$ ARE LINEARLY PROPORTIONAL TO $Z$. IN REACTING CONDITIONS, THE SOLUTION TO (6) REDUCES TO THE SOLUTION OF $\rho\chi\dfrac{\partial^2 T}{\partial Z^2} = -\dfrac{q S W_F}{c_p}\dot{\omega}$ TOGETHER WITH (3) AND (4), AND WITH $\chi(Z)$ GIVEN BY THE SOLUTION TO (1).

WHEN THE FROZEN PROFILES $Y_F = Y_{F,F}\,Z$ AND $Y_{O_2} = Y_{O_2,A}(1-Z)$ ARE USED IN THE DEFINITION OF THE EQUIVALENCE RATIO $\phi = \dfrac{S Y_F}{Y_{O_2}}$, THE RELATION

NOTICE THAT $\phi = 1$ AT $Z = Z_{st}$

$$\phi = \frac{(1-Z_{st})}{Z_{st}}\frac{Z}{1-Z}$$

IS OBTAINED, WHICH IS VALID ONLY WHEN $D_F$ AND $D_{O_2}$ ARE EQUAL.

EQUATIONS (1) AND (2) CAN STILL BE USED WHEN THE CHEMISTRY IS FAST AND COMBUSTION OCCURS IN THIN REACTION LAYERS, WITH ALL INTERMEDIATES IN STEADY STATE.

A MORE GENERAL WAY OF DEFINING THE MIXTURE FRACTION INVOLVES CHEMICAL ELEMENTS INSTEAD OF SPECIES. WHILE THE MASS OF CHEMICAL SPECIES MAY CHANGE DUE TO CHEMICAL REACTIONS, THE MASS OF ELEMENTS IS CONSERVED. FOR INSTANCE, $CH_4$ HAS TWO ELEMENTS ($C + H$). THE MASS FRACTION OF THE ELEMENT $k$ CAN BE OBTAINED AS

$$Z_k = \frac{m_k}{m} = \sum_{i=1}^{N}\frac{a_{k,i}W_k}{W_i}Y_i, \quad \text{WITH } a_{k,i} \text{ THE TOTAL NUMBER OF ATOMS } k \text{ IN SPECIES } i.$$

SINCE THE MASS OF ELEMENTS IS CONSERVED, THEN $\sum_{i=1}^{N} a_{k,i}\left(\nu''_{i,j} - \nu'_{i,j}\right) = 0$ FOR REACTION $j$. FOR EVERY SPECIES $i$, A CONSERVATION EQUATION OF THE TYPE

$$\rho\frac{\partial Y_i}{\partial t} + \rho\,\underline{v}\cdot\nabla Y_i = \nabla\cdot(\rho D_i \nabla Y_i) + \dot{w}_i$$

CAN BE WRITTEN. MULTIPLYING THIS EQUATION BY $a_{k,i}W_k/W_i$ AND SUMMING OVER ALL SPECIES, THE CONSERVATION EQUATION

$$\rho\frac{\partial Z_k}{\partial t} + \rho\,\underline{v}\cdot\nabla Z_k = \nabla\cdot(\rho D\nabla Z_k) + \sum_{i=1}^{N}\frac{a_{k,i}W_k}{W_i}\dot{w}_i \qquad (7)$$

WITH THE LAST TERM VANISHING SINCE $\sum_{i=1}^{N}\frac{a_{k,i}W_k}{W_i}\dot{w}_i = \sum_{i=1}^{N}\frac{a_{k,i}W_k}{W_i}\sum_{j=1}^{M}W_i\left(\nu''_{i,j} - \nu'_{i,j}\right)\dot{\omega}_j = 0$, $i = 1,\dots N$.

NOTE THAT IN (7) IT HAS BEEN ASSUMED THAT ALL DIFFUSIVITIES OF THE SPECIES ARE EQUAL $D_i = D$.

BY NOTICING THAT $\frac{Z_C}{mW_C} = \frac{Z_H}{nW_H} = \frac{Y_{F,F}}{W_F}$ IN THE FUEL STREAM AND $Z_O = Y_{O_2,A}$,

A MIXTURE FRACTION $Z = \dfrac{Z_C/mW_C + Z_H/nW_H + Z(Y_{O_2,A} - Z_O)/bW_{O_2}}{Z Y_{F,F}/W_F + Z\,Y_{O_2,A}/bW_{O_2}}$ CAN BE DEFINED, WHICH SATISFIES $Z = 0$ IN THE OXIDIZER STREAM AND $Z = 1$ IN THE FUEL STREAM, WITH $Z = Z_{st}$ AT STOICHIOMETRY.

*NOTE ON $D_F \neq D_{O_2}$: THESE ANALYSES CAN BE GENERALIZED FOR NON-EQUIDIFFUSIVE FLAMES (SEE PITSCH+PETERS, 1998) BY DEFINING $Z$ AS A SCALAR GIVEN BY (1) / OR BY USING 2 MIXTURE FRACTIONS (SELIÑA'N ET AL, 1994)

## THE BURKE-SCHUMANN SOLUTIONS

IN THE BURKE SCHUMANN LIMIT (SEE PAGE 9), THE DAMKÖHLER NUMBER IS LARGE AND THE CHEMICAL REACTION IS CONFINED TO A (INFINITESIMALLY) THIN REGION AROUND $Z = Z_{st}$, WHICH SEPARATES A FUEL-ONLY ZONE FROM AN OXIDIZER-ONLY ZONE. IN THIS LIMIT, THE SPECIES CONSERVATION EQUATIONS REDUCE TO $Y_{O_2} Y_F \to 0$ IN THE FIRST APPROXIMATION IN $\Delta$. THEREFORE, THE FUEL AND OXIDIZER PROFILES CAN BE OBTAINED BY IMPOSING $Y_F = 0$ AND $Y_{O_2} = 0$ IN (3) AND (4), RESPECTIVELY:

$$T = T_{O_2,A} + (T_{F,F} - T_{O_2,A}) Z + \frac{q}{c_p} \frac{s Y_{F,F}}{} Z$$

$$Y_F = 0$$

$$Y_{O_2} = Y_{O_2,A} \left( 1 - \frac{Z}{Z_{st}} \right)$$

ON THE OXIDIZER SIDE $Z < Z_{st}$

AND

$$T = T_{O_2,A} + (T_{F,F} - T_{O_2,A}) Z + \frac{q}{c_p} Y_{O_2,A} (1 - Z)$$

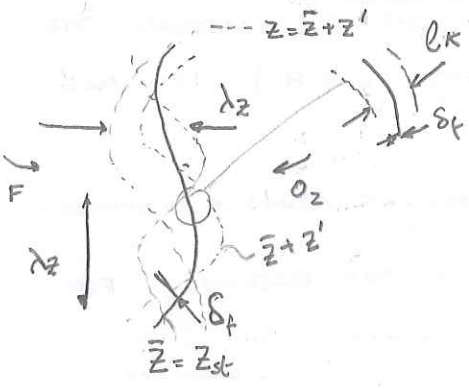
$$Y_F = Y_{F,F} \frac{Z - Z_{st}}{1 - Z_{st}}$$

$$Y_{O_2} = 0$$

ON THE FUEL SIDE $Z > Z_{st}$

⇒ DEPARTURES FROM EQUILIBRIUM (I.E. BURKE-SCHUMANN) TYPICALLY OCCUR IN REAL FLAMES (SEE FIGS 1 AND 2)

## THE FLAMELET ASYMPTOTIC LIMIT (NON PREMIXED)




A TAYLOR LENGTH SCALE $\lambda_Z$ FOR THE MIXTURE FRACTION $Z$ CAN BE DEFINED AS THE CHARACTERISTIC THICKNESS OF THE ZONES IN WHICH MOLECULAR DIFFUSION IS IMPORTANT IN AN AVERAGE SENSE,

$$\bar{\chi}_{st} = D \overline{|\nabla Z|^2}_{st} \sim D \frac{\overline{Z'^2}_{st}}{\lambda_Z^2} \to \lambda_Z \sim \frac{(\overline{Z'^2})^{1/2}_{st}}{\overline{|\nabla Z|}_{st}}, \text{ WITH } \lambda_Z \gg \ell_K$$

THE FLAME THICKNESS, AS OBSERVED IN PAGE 10, CAN BE OBTAINED FROM THE CHARACTERISTIC MIXTURE-FRACTION VARIATIONS ACCROSS THE FLAME

$$\Delta Z)_f \sim Z - Z_{st} \sim \frac{\Delta^{-1/3}}{\beta} Z_{st} \to \delta_f = \frac{\Delta Z)_f}{|\nabla Z|_{st}} \sim \frac{\Delta^{-1/3}}{\beta} \cdot \left( \frac{D_T}{\chi_{st}} \right)^{1/2} Z_{st}$$

$$\to \delta_f \sim \frac{\Delta^{-1/3}}{\beta} \ell_K, \text{ WITH } \ell_K \sim \left( \frac{D_T}{a} \right)^{1/2} \text{ THE KOLMOGOROV LENGTH (HERE } S_c = 1 \text{ HAS BEEN USED)}.$$

IN THIS FORMULATION, THE APPROXIMATION $\chi_{st} \sim a Z_{st}^2$ HAS BEEN USED, SINCE $Z = \frac{1}{2} \operatorname{erfc}\left( \frac{z}{\sqrt{2}} \right) \sim \frac{1}{\sqrt{2\pi}} \frac{e^{-z^2/2}}{z}$ FOR LARGE $z$, AND $\chi = a \left( \frac{dZ}{dz} \right)^2 =$ (DIMENSIONLESS $z = z/\ell_K$)

$$= \frac{a}{2\pi} \left[ -e^{-\frac{z^2}{2}} + \frac{e^{-z^2/2}}{z^2} \right]^2 \sim a Z^2 z^2 \sim 2a Z^2 \underbrace{\operatorname{erfc}^{-1}(2Z^2)}_{O(1) \text{ WHEN } Z \to Z_{st}} \Rightarrow \chi_{st} \sim 2a Z_{st}^2 \quad \text{FOR } Z_{st} \ll 1$$

(MUCH SMALLER)

THE FLAMELET LIMIT IS APPROACHED WHEN $\varepsilon = \frac{\delta_f}{\lambda_Z} \propto \delta_f \frac{\overline{|\nabla Z|}_{st}}{(\overline{Z'^2})^{1/2}} \ll 1 \Rightarrow$ WHEN DIFFUSION LAYER WHERE THE MEAN FLAME REGION SITS IS MUCH LARGER THAN THE REACTION LAYER THICKNESS

⇒ GIVEN THE SPECIES CONSERVATION EQUATION $\rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla Y_i = \nabla \cdot (\rho D \nabla Y_i) + \dot{w}_i$

AND NONDIMENSIONALIZING ($\lambda_z$: OUTER SCALES) $\underline{x}^* = \underline{x}/\lambda_z$, $t^* = t/\lambda_z^2/D_{st}$, $\underline{v}^* = \underline{v}\,\lambda_z/D_{st}$, $\rho^* = \rho/\rho_0$

$\dot{w}_i^{*} = \dot{w}_i / \rho_0 D_{st}/\lambda_z^2$, THEN THE SPECIES CONSERVATION EQUATION

REMAINS THE SAME: $\rho \frac{\partial Y_i}{\partial t} + \rho \underline{v} \cdot \nabla Y_i = \nabla \cdot (\rho D \nabla Y_i) + \dot{w}_i$. (DROPPING $^*$)

SINCE $\frac{\Delta Z)_f}{(\overline{Z''^2})^{1/2}_{st}} \sim \frac{\delta_f |\nabla Z|_{st}}{(\overline{Z''^2})^{1/2}_{st}} \sim \varepsilon \ll 1$, THEN AN "INNER" MIXTURE FRACTION $\eta$ CAN BE

DEFINED AS $\eta = \frac{Z - Z_{st}}{(\overline{Z''^2})^{1/2}\varepsilon} = \hat{Z}/\varepsilon$, WHICH BECAMES $\eta = O(1)$ IN THE REACTION ZONE.

THEN $\frac{\partial}{\partial t} = \frac{\partial \hat{Z}}{\partial t}\frac{\partial}{\partial \hat{Z}} + \frac{\partial}{\partial \tau}$, $\nabla = \nabla \hat{Z}\frac{\partial}{\partial \hat{Z}} + \nabla_\perp$ AND THE SPECIES EQUATION BECOMES:

$$\rho \frac{\partial Y_i}{\partial t} + \left[\rho \frac{\partial \hat{Z}}{\partial t} + \rho \underline{v} \cdot \nabla \hat{Z}\right] \frac{\partial Y_i}{\partial \hat{Z}} + \rho \underline{v} \cdot \nabla_\perp Y_i =$$

$$= \nabla \hat{Z} \frac{\partial}{\partial \hat{Z}}\left(\rho D \nabla \hat{Z} \frac{\partial Y_i}{\partial \hat{Z}}\right) + \nabla \hat{Z} \frac{\partial}{\partial \hat{Z}}\left(\rho D \nabla_\perp Y_i\right) + \nabla_\perp \cdot \left(\rho D \nabla_\perp Y_i\right)$$

$$+ \nabla_\perp \cdot \left(\rho D \nabla \hat{Z} \frac{\partial Y_i}{\partial \hat{Z}}\right) + \dot{w}_i$$

INTRODUCING THE INNER MIXTURE FRACTION $\eta$ IN THE EQUATION ABOVE, ONE OBTAINS:

$$\rho \frac{\partial Y_i}{\partial t} + \frac{1}{\varepsilon}\left[\rho \frac{\partial \hat{Z}}{\partial t} + \rho \underline{v} \cdot \nabla \hat{Z}\right] \cdot \frac{\partial Y_i}{\partial \eta} + \rho \underline{v} \cdot \nabla_\perp Y_i = \frac{1}{\varepsilon^2} \nabla \hat{Z} \frac{\partial}{\partial \eta}\left(\rho D \nabla \hat{Z} \frac{\partial Y_i}{\partial \eta}\right) + \frac{1}{\varepsilon} \nabla \hat{Z} \frac{\partial}{\partial \eta}\left(\rho D \nabla_\perp Y_i\right)$$

$$+ \nabla_\perp \cdot \left(\rho D \nabla_\perp Y_i\right) + \frac{1}{\varepsilon} \nabla_\perp \cdot \left(\rho D \nabla \hat{Z} \frac{\partial Y_i}{\partial \eta}\right) + \dot{w}_i$$

SINCE $\rho \frac{\partial \hat{Z}}{\partial t} + \rho \underline{v} \cdot \nabla \hat{Z} = \nabla \cdot (\rho D \nabla \hat{Z}) = \frac{1}{\varepsilon} \nabla \hat{Z} \frac{\partial}{\partial \eta}\left(\rho D \nabla \hat{Z}\right)$, THEN THE ABOVE EQUATION

REDUCES TO $\rho D |\nabla \hat{Z}|^2 \frac{\partial^2 Y_i}{\partial \eta^2} = -\dot{w}_i'$ TO ORDER $\frac{1}{\varepsilon^2}$, WHERE $\dot{w}_i' = w_i \varepsilon^2$ HAS

(WITH THIS THE CHEMICAL TIME BECOMES $\delta_f^2/D$)

BEEN RESCALED TO RETAIN THE REACTION TERM. IN ORIGINAL VARIABLES, THE RESULTING FLAMELET

PROBLEM BECOMES $\rho D |\nabla Z|^2 \frac{\partial Y_i}{\partial Z^2} = -\dot{w}_i$, OR EQUIVALENTLY: $\boxed{\rho \chi \frac{\partial^2 Y_i}{\partial Z^2} = -\dot{w}_i}$

WHERE $\chi = D|\nabla Z|^2$ IS THE SCALAR DISSIPATION RATE. NOTE THAT UNSTEADY TERMS

HAVE BEEN NEGLECTED SINCE THEY HAVE BEEN SCALED WITH THE OUTER TIME $\lambda_z^2/D$.

IN FACT, ONE NEEDS TIME VARIATIONS OF ORDER $\varepsilon^2 \lambda_z^2/D = \delta_f^2/D$, WHICH, CLOSE TO

EXTINCTION, BECOME OF ORDER $\tau_K/\beta^2$ (PERTURBATIONS ACTING ON TIMES $> \frac{\tau_R}{\beta^2}$ ARE IRRELEVANT IN

THE REACTION ZONE).

EQUIVALENCE BETWEEN PREMIXED AND DIFFUSION FLAMES

IF THE ANALYSIS OF PAGE 8 FOR PREMIXED FLAMES WAS TO BE REPEATED FOR 2 REACTANTS NEAR STOICHIOMETRY, ONE WOULD OBTAIN $S_{L,st}^0 = \left(\frac{4AD_T}{\beta^3} Y_{O_2,st}\, e^{-T_a/\hat{T}_b}\right)^{1/2}$, WITH $Y_{O_2 st} = Y_{O_2,A}(1 - Z_{st})$. ($\hat{T}_b$: ADIABATIC TEMPERATURE) ~ SEE (MITANI, 1980)

FROM THE EXTINCTION CONDITION IN DIFFUSION FLAMES (PAGE 10), IT WAS FOUND THAT

$\Delta_E \sim \frac{4 Z_{st}^2 (1 - Z_{st})^2 Y_{O_2,st} A\, e^{-T_a/T_b}}{\chi_q \beta^3} \sim e^{-1}$, SO THAT $\frac{Z_{st}^2 (1 - Z_{st})^2 S_{L,st}^{0\,2}/D_T}{\chi_q} \sim 1$ → UPON EXTINCTION → $\boxed{\frac{Z_{st}^2 (1 - Z_{st})^2}{t_F} = \chi_q}$

($\chi_q$ = EXTINCTION SCALAR DISS. RATE; $t_F = \delta_L^2/D_T$ → FLAME TRANSIT TIME)

NOTICE THAT THIS EXPRESSION CAN BE WRITTEN IN THE FOLLOWING DIFFERENT WAY. SINCE $\chi_q \sim a_q Z_{st}^2$ FOR $Z_{st}$ SMALL, WITH $a_q$ THE EXTINCTION STRAIN RATE, THEN, $\delta_M \sim l_K$

$$\chi_q = \frac{Z_{st}^2 (1-Z_{st})^2}{t_F} \rightarrow a_q Z_{st}^2 = \frac{Z_{st}^2 (1-Z_{st})^2}{\delta_L^{02}/D_T} \rightarrow (1-Z_{st})^2 \frac{\delta_M^2}{\delta_L^2} \sim \boxed{\frac{\delta_M^2}{\delta_L^2} \sim 1} \quad \text{AT EXTINCTION}$$

WITH $\delta_M \sim \left(D_T/a_q\right)^{1/2}$ A MIXING-LAYER THICKNESS, WHICH IN TURBULENT COMBUSTION PLAYS THE ROLE OF A KOLMOGOROV THICKNESS $l_K$. $\Rightarrow$ AT DIFFUSION-FLAME EXTINCTION, THE THICKNESS OF THE MIXING LAYER EQUALS THE THICKNESS OF THE LAMINAR PREMIXED FLAME.

WHILE IN LAMINAR PREMIXED FLAMES THERE IS ONLY ONE TIME SCALE, (THE FLAME-TRANSIT TIME $t_F$), IN DIFFUSION FLAMES THERE EXISTS A FUNDAMENTAL BALANCE BETWEEN THE DIFFUSION TIME THROUGH THE STOICHIOMETRIC SURFACE $\chi_{st}^{-1}$ (NOTE THAT, SINCE $\chi_{st} \sim a Z_{st}^2$ FOR $Z_{st} \ll 1$, THEN $\chi_{st}^{-1} \gg 1/a$, OR EQUIVALENTLY, THE STOICHIOMETRIC SCALAR DISSIPATION RATE CAN BE MUCH SMALLER THAN THE STRAIN RATE) AND THE LOCAL CHEMICAL TIME $t_c \sim \left(\frac{A Y_{O_2,st}}{\beta^2} e^{-T_a/T_b}\right)^{-1}$, WITH $\Delta = 1/t_c \chi_{st}$ A DAMKÖHLER NUMBER.

## MODELLING NON-PREMIXED TURBULENT COMBUSTION

MODELS IN NONPREMIXED COMBUSTION ARE OFTEN BASED ON THE PRESUMED-SHAPE PDF, WHICH REQUIRES KNOWLEDGE OF $\tilde{Z}$ AND $\widetilde{Z''^2}$. THE FAVRE-AVERAGED EQUATIONS FOR $\tilde{Z}$ AND $\widetilde{Z''^2}$ ARE

$$\bar{\rho}\frac{\partial \tilde{Z}}{\partial t} + \bar{\rho}\underline{\tilde{v}} \cdot \nabla \tilde{Z} = -\nabla \cdot \left(\bar{\rho}\,\widetilde{\underline{v}''Z''}\right) \qquad (1)$$

$$\bar{\rho}\frac{\partial \widetilde{Z''^2}}{\partial t} + \bar{\rho}\underline{\tilde{v}} \cdot \nabla \widetilde{Z''^2} = -\nabla \cdot \left(\bar{\rho}\,\widetilde{\underline{v}''Z''^2}\right) - 2\bar{\rho}\,\widetilde{v''Z''}\nabla\tilde{Z} - 2\bar{\rho}\tilde{\chi} \qquad (2)$$

WITH $\widetilde{\underline{v}''Z''}$ USUALLY MODELLED BY EMPLOYING THE GRADIENT-HYPOTHESIS (NOTICE HOWEVER THAT THERE CAN BE COUNTERGRADIENT DIFF. ↳ SEE LUO+BRAY (1998)) $\widetilde{v''Z''} = -D_t \nabla \tilde{Z}$, AND WITH $\tilde{\chi} = D\left|\nabla Z''\right|^2$ THE SCALAR DISSIPATION RATE. IN ADDITION TO THESE EQUATIONS, ONE NEEDS CONTINUITY, MOMENTUM, SPECIES OR ENERGY CONSERVATION EQUATIONS ARE REQUIRED TO CLOSE THE SYSTEM. THE SCALAR DISSIPATION RATE IS TYPICALLY MODELLED BY USING THE EXPRESSION $\tilde{\chi} = C_\chi \frac{\varepsilon}{\kappa} \widetilde{Z''^2}$, WITH $C_\chi$ A CONSTANT, OR BY SOLVING A TRANSPORT EQUATION FOR $\tilde{\chi}$.

THERE ARE 2 MAIN APPROACHES FOR MODELLING NON-PREMIXED COMBUSTION:

a) IN THE FIRST APPROACH, THE FORMULATION CONSISTS OF (1), (2) PLUS THE CONTINUITY AND MOMENTUM EQUATIONS. THE SPECIES MASS FRACTIONS AND TEMPERATURE ARE OBTAINED FROM

$$\bar{\rho}\tilde{Y}_i = \int_0^1 \langle \rho Y_i \,|\, Z \rangle P(Z)\, dZ \quad \text{AND} \quad \bar{\rho}\tilde{T} = \int_0^1 \langle \rho T \,|\, Z \rangle P(Z)\, dZ$$

WHERE $\langle \rho\phi \,|\, Z \rangle$ REFERS TO THE CONDITIONAL MEAN OF $\rho\phi$ FOR A GIVEN VALUE OF $Z$, AND $P(Z)$ IS THE PROBABILITY DENSITY FUNCTION OF $Z$. THE MAGNITUDES $\langle \rho\phi \,|\, Z \rangle$ ARE OBTAINED TYPICALLY FROM INFINITELY-FAST CHEMISTRY ASSUMPTIONS OR FROM FLAMELET LIBRARIES.

IN COMPUTATIONS, A TWO-PARAMETER PDF IS PRESUMED IN ADVANCE, WHICH TYPICALLY CONSISTS OF A BETA PDF:

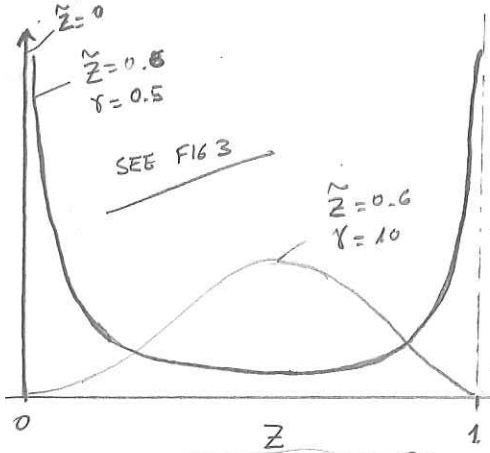
$$P(Z;\alpha,\beta) = \frac{Z^{\alpha-1}(1-Z)^{\beta-1}\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}$$

WITH $\Gamma$ THE GAMMA FUNCTION AND $\alpha$ AND $\beta$ GIVEN BY

$$\alpha = \tilde{Z}\gamma \quad , \quad \beta = (1-\tilde{Z})\gamma$$

WHERE $\gamma = \frac{\tilde{Z}(1-\tilde{Z})}{\widetilde{Z''^2}} - 1 \qquad \left(0 \le \widetilde{Z''^2} \le \tilde{Z}(1-\tilde{Z})\right)$

WHICH SATISFIES $\tilde{Z} = \int_0^1 Z P(Z)\,dZ$ AND $\widetilde{Z''^2} = \int_0^1 (Z-\tilde{Z})^2 P(Z)\,dZ$.




⇒ IT FAILS IN JETS AND SHEAR FLOWS ACCROSS THE VISCOUS SUPERLAYER ↓ SEE FIG 4 AND EFFELSBERG + PETERS (1983)

→ NEEDS $\tilde{Z}$ AND $\widetilde{Z''^2}$ AS PARAMETERS CALCULATED FROM THE $\tilde{Z}$ AND $\widetilde{Z''^2}$ EQUATIONS (1) AND (2)

NOTICE THAT AT $\tilde{Z}=0$ OR $\tilde{Z}=1$ THE PDF DEGENERATES INTO A DELTA FUNCTION.

- FOR THE CASE IN WHICH THE FLAME IS ASSUMED TO BE IN THE INFINITELY-FAST CHEMISTRY LIMIT, THE EXPRESSIONS $Y_F(Z)$, $Y_{O_2}(Z)$ AND $T(Z)$ GIVEN FOR THE BURKE-SCHUMANN SOLUTIONS (SEE BACK PAGE 24) CAN BE USED TO MODEL $\langle \rho Y_i | Z\rangle$ AND $\langle \rho T | Z\rangle$, SINCE

$$\langle \rho\phi | Z\rangle = \int_0^1 \rho\phi\, P(\rho\phi|Z)\,dZ, \quad \text{WITH} \quad P(\rho\phi|Z) = \frac{P(\rho\phi, Z)}{P(Z)} = \delta(\rho\phi - \rho\phi(Z))$$

THEN $\langle \rho\phi | Z\rangle = \rho(Z)\phi(Z) \rightarrow \langle \rho Y_i | Z\rangle = \rho(Z) Y_i(Z)$ AND $\langle \rho T | Z\rangle = \rho(Z) T(Z)$.

THEN $\bar{\rho}\tilde{Y}_i = \int_0^1 \rho(Z) Y_i(Z) P(Z)\,dZ$ AND $\bar{\rho}\tilde{T} = \int_0^1 \rho(Z) T(Z) P(Z)\,dZ$, WHICH CAN BE EXPRESSED IN TERMS OF THE FAVRE-AVERAGED PDF: $\tilde{P}(Z) = \int_0^\infty \rho P(\rho, Z)\frac{d\rho}{\bar{\rho}} = \int_0^\infty \rho P(Z) \underbrace{P(\rho|Z)}_{\delta(\rho-\rho(Z))} dZ = \rho(Z) P(Z)/\bar{\rho}$

AS $\tilde{Y}_i = \int_0^1 Y_i(Z)\tilde{P}(Z)\,dZ$ AND $\tilde{T} = \int_0^1 T(Z)\tilde{P}(Z)\,dZ$. SEE FIG 5 FOR SCHEMATICS.

- FOR CASES IN WHICH FINITE-RATE CHEMISTRY EFFECTS ARE RETAINED, A FLAMELET APPROACH IS TYPICALLY USED. IN THE FLAMELET LIMIT, THE REACTION ZONE THICKNESS IS SMALLER THAN A KOLMOGOROV EDDY, AND COMBUSTION OCCURS IN A QUASI-LAMINAR FLOW IN THE FLAME REGION, WHICH IS DESCRIBED BY THE FLAMELET EQUATION $\rho\chi\frac{\partial^2\phi}{\partial Z^2} = -\dot{w}_\phi$, $\phi = Y_i, T$. IN THIS APPROACH, THE FLAMELET SOLUTIONS $Y_i(Z,\chi_{st})$, $T(Z,\chi_{st})$ ARE STORED IN TABLES. THE MEAN SPECIES MASS FRACTIONS AND TEMPERATURE ARE CALCULATED FROM

$$\bar{\rho}\tilde{Y}_i = \int_0^{+\infty}\int_0^1 \rho Y_i(Z,\chi_{st}) P(Z,\chi_{st})\,dZ\,d\chi_{st} \quad \text{AND} \quad \bar{\rho}\tilde{T} = \int_0^{+\infty}\int_0^1 \rho T(Z,\chi_{st}) P(Z,\chi_{st})\,dZ\,d\chi_{st}.$$

WHEN STATISTICAL INDEPENDENCE IS ASSUMED BETWEEN THE MIXTURE FRACTION AND THE SCALAR DISSIPATION RATE, THEN $P(Z,\chi_{st}) = P(Z)P(\chi_{st})$, WITH $P(Z)$ GIVEN BY THE BETA PDF AND $P(\chi_{st})$ IS USUALLY APPROXIMATED BY A DELTA FUNCTION $P(\chi_{st}) = \delta(\chi_{st} - \tilde{\chi}_{st})$. WHILE $\tilde{\chi}$ CAN BE CALCULATED BY USING CLOSURE METHODS OR BY SOLVING A TRANSPORT EQUATION, AS DESCRIBED ABOVE. THE STOICHIOMETRIC SCALAR DISSIPATION RATE CAN BE OBTAINED BY USING THE EXPRESSION:

$\tilde{\chi}_Z = \frac{a}{2\pi} e^{-2[\mathrm{erfc}^{-1}(2Z)]^2}$ FOR THE CONDITIONAL SCALAR DISSIPATION RATE, WHICH LEADS TO

$$\tilde{\chi}_Z = \tilde{\chi}_{st} \frac{e^{-2[\mathrm{erfc}^{-1}(2Z)]^2}}{e^{-2[\mathrm{erfc}^{-1}(2Z_{st})]^2}} = \tilde{\chi}_{st} \frac{f(Z)}{f(Z_{st})}, \quad \text{SO THAT} \quad \tilde{\chi} = \int_0^1 \tilde{\chi}_Z \tilde{P}(Z)\,dZ = \tilde{\chi}_{st} \int_0^1 \frac{f(Z)}{f(Z_{st})} \tilde{P}(Z)\,dZ.$$

USING THIS EXPRESSION, THE CONDITIONAL FAVRE MEAN SCALAR DISSIPATION RATE $\tilde{\chi}_{st}$ IS

$$\tilde{\chi}_{st} = \frac{\tilde{\chi} f(Z_{st})}{\int_0^1 f(Z) P(Z) dZ}, \quad \text{WHICH CAN BE USED HERE TO CALCULATE } \tilde{\chi}_Z.$$

SEE FIGURE FOR SCHEMATICS.

ii) IN THE SECOND APPROACH, TRANSPORT EQUATIONS FOR $\tilde{T}$ AND $\tilde{Y}_i$ ARE SOLVED, WITH THE MEAN REACTION TERM $\overline{\dot{w}}_i$ BEING READ FROM THE FLAMELET LIBRARY. THEN

$$\overline{\dot{w}}_i = \int_0^1 \int_0^\infty \dot{w}_i(Z, \chi_{st}) P(Z, \chi_{st})\, dZ\, d\chi_{st},$$

WITH $\dot{w}_i(Z, \chi_{st})$ TABULATED AND $\tilde{\chi}_{st}$ OBTAINED, FOR INSTANCE, AS OUTLINED ABOVE.

→ SEE FIG. 6 FOR SCHEMATICS

THE FLAMELET PROGRESS-VARIABLE APPROACH. (PIERCE + MOIN, 2004)

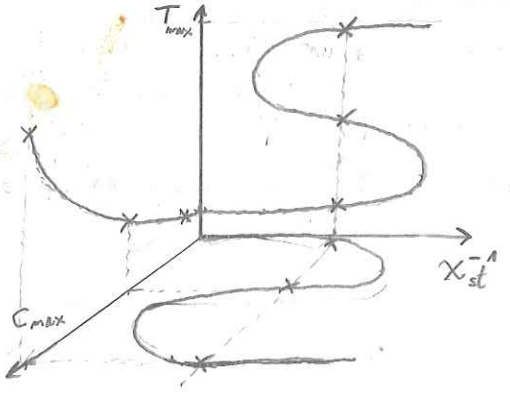
THE LES EQUATIONS FOR REACTING FLOWS ARE

$$\begin{cases} \frac{\partial \bar{\rho}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}) = 0 \\ \frac{\partial}{\partial t}(\bar{\rho}\tilde{\underline{u}}) + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{\underline{u}}) = -\nabla\bar{p} + \nabla\cdot\left[\bar{\underline{\tau}} - \bar{\rho}(\widetilde{\underline{u}\underline{u}} - \tilde{\underline{u}}\tilde{\underline{u}})\right] \\ \frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{Y}_i) = \nabla\cdot\left[\bar{\rho}\,\overline{\underline{V}_i Y_i} - \bar{\rho}(\widetilde{\underline{u} Y_i} - \tilde{\underline{u}}\tilde{Y}_i)\right] + \overline{\dot{w}}_i \\ \frac{\partial}{\partial t}(\bar{\rho}\tilde{h}_s) + \nabla\cdot(\bar{\rho}\tilde{\underline{u}}\tilde{h}_s) = \frac{\overline{Dp}}{Dt} + \nabla\cdot\left[\overline{\lambda\nabla T} - \bar{\rho}(\widetilde{\underline{u} h_s} - \tilde{\underline{u}}\tilde{h}_s)\right] + \overline{\underline{\tau}:\nabla\underline{u}} - \nabla\cdot\left(\overline{\rho\sum_{i=1}^{N}\underline{V}_i Y_i h_{s_i}}\right) - \sum_{i=1}^{N}\overline{h_i^o \dot{w}_i^o} \end{cases}$$

WHERE $\bar{\ }$ AND $\tilde{\ }$ DENOTE FILTERED AND FAVRE-FILTERED VARIABLES. NOTICE THAT THE SUBGRID FLUXES $\bar{\rho}(\widetilde{\underline{u}\phi} - \tilde{\underline{u}}\tilde{\phi})$, THE PRESSURE VELOCITY TERM $\overline{\frac{Dp}{Dt}}$, THE RAYLEIGH DISSIPATION $\overline{\underline{\tau}:\nabla\underline{u}}$ AND THE FILTERED REACTION RATE $\overline{\dot{w}_i}$ NEED MODELLING. SINCE COMBUSTION REQUIRES REACTANTS TO BE MIXED AT THE MOLECULAR LEVEL, CHEMICAL REACTIONS OCCUR AT THE SUBGRID LEVEL.

THE FLAMELET PROGRESS-VARIABLE APPROACH (FPVA IN WHAT FOLLOWS) WAS DESIGNED TO DEAL WITH FLAME LIFT-OFF IN NON-PREMIXED COMBUSTION, IN AN ATTEMPT TO MODEL LIFT OFF BY USING THE LOWER TURNING POINT OF THE S-CURVE.

THE SUBGRID TURBULENT FLUXES CAN BE CLOSED BY USING TECHNIQUES OUTLINED IN PAGE 15.

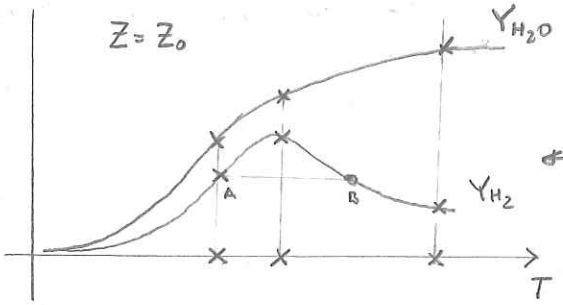



NOTE THAT A PARAMETRIZATION $T(Z, \chi_{st})$, $Y_i(Z, \chi_{st})$ INVOLVES MULTIVALUED SOLUTIONS: FOR EACH VALUE OF $\chi_{st}$ THERE EXIST 3 VALUES OF $T$ AND $Y_i$. IN THE FPVA MODEL, A DIFFERENT TABULATION STRATEGY IS PROPOSED:

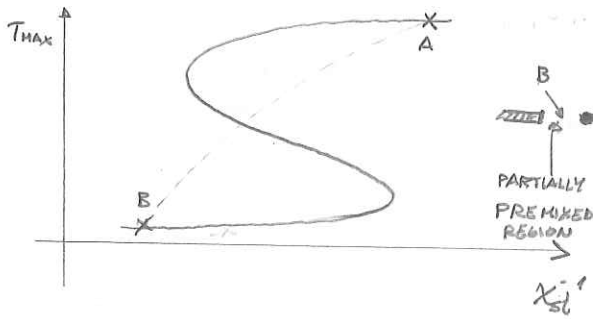
$$T = T(Z, C), \text{ AND } Y_i(Z, C)$$

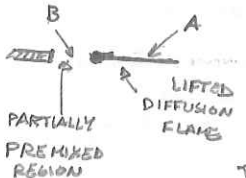
WITH $C$ A PROGRESS VARIABLE THAT PROVES TO PROVIDE A UNIQUE MAPPING OF ALL THE CHEMICAL STATES IN THE FLAMELET LIBRARY (IN CONTRAST WITH $\chi_{st}$),

WHEN PARAMETRIZATION IS MADE IN TERMS OF $\tilde{Z}$ AND $\chi_{st}$, AS IN STEADY FLAMELETS (SEE PREVIOUS SECTION) THERE IS NO ACCESS TO SOLUTIONS IN THE IGNITION BRANCH OR IN THE PARTIAL BURNING BRANCH (ALTHOUGH THE LATTER ONE HAS BEEN PROVED TO BE UNSTABLE). IF THE PROGRESS VARIABLE $C$ IS CHOSEN IN SUCH A MANNER THAT IT PROVIDES A UNIQUE MAPPING OF $\phi = \phi(Z,C)$ FOR EVERY $Z$ AND SCALAR $\phi$, THEN THE PROFILES $\phi(Z,C)$ STORED IN THE FLAMELET TABLES FOR THE ENTIRE $S$ CURVE CAN BE RETRIEVED UNIVOCALLY GIVEN $\tilde{Z}$ AND $C \Rightarrow$ WITH THIS ONE CAN HAVE ACCESS TO THE IGNITION, PARTIAL-BURNING AND EXTINCTION BRANCHES.




EX: IF $C = Y_{H_2O}$ THEN FOR EACH $C$, ONE CAN RETRIEVE A SINGLE VALUE OF $Y_{H_2}$ AND $T$. HOWEVER, IF $C = Y_{H_2O}$, THERE WOULD BE TWO SAME $C$'s (A AND B) GIVING DIFFERENT VALUES OF $T$ AND $Y_{H_2O} \Rightarrow$ NOT A GOOD CHOICE FOR $C$. THE PROGRESS VARIABLE TENDS TO BE CHOSEN TO BE THE PRODUCT MASS FRACTION OR A SUITABLE COMBINATION OF MASS FRACTIONS SUCH AS THE MAPPING IS UNIQUE.




THE FPVA MODEL ATTEMPTS TO HAVE ACCESS TO THE IGNITION BRANCH IN ORDER TO DESCRIBE THE CHEMICALLY FROZEN REGION B IN LIFTED DIFFUSION FLAMES. IT SHOULD BE NOTED HOWEVER THAT THE STRUCTURES OF THIS REGION B AND OF THE EDGE DEVELOPED BETWEEN A AND B DIFFER CONSIDERABLY FROM THE PHYSICS DESCRIBED BY THE LOWER BRANCH OF THE $S$ CURVE, NOR THE PATH B→A CAN BE DESCRIBED BY THE USE OF NON-PREMIXED FLAMELETS.

WHEN THE PROGRESS VARIABLE $C$ HAS BEEN CHOSEN, THE ENTHALPY AND SPECIES CONSERVATION EQUATIONS ARE RULED OUT IN FAVOR OF THE EQUATIONS

$$\left.\begin{aligned} \frac{\partial}{\partial t}\left(\bar{\rho}\tilde{Z}\right) + \nabla\cdot\left(\bar{\rho}\tilde{\underline{u}}\tilde{Z}\right) &= \nabla\cdot\left[\bar{\rho}\left(D + D_t\right)\nabla\tilde{Z}\right] \\ \frac{\partial}{\partial t}\left(\bar{\rho}\tilde{C}\right) + \nabla\cdot\left(\bar{\rho}\tilde{\underline{u}}\tilde{C}\right) &= \nabla\cdot\left[\bar{\rho}\left(D + D_t\right)\nabla\tilde{C}\right] + \bar{\dot{w}}_C \end{aligned}\right\}$$

FOR $\tilde{Z}$ AND $C$, WHERE $D_t$ IS A TURBULENT DIFFUSIVITY. THE FILTERED SPECIES MASS FRACTIONS AND TEMPERATURE CAN THEN BE OBTAINED FROM

$$\tilde{Y}_i = \int_0^1\int_0^1 Y_i(Z,C)\,\tilde{P}(Z,C)\,dZ\,dC \qquad \tilde{T} = \int_0^1\int_0^1 T(Z,C)\,\tilde{P}(Z,C)\,dZ\,dC$$

AND THE FILTERED SOURCE TERM AS

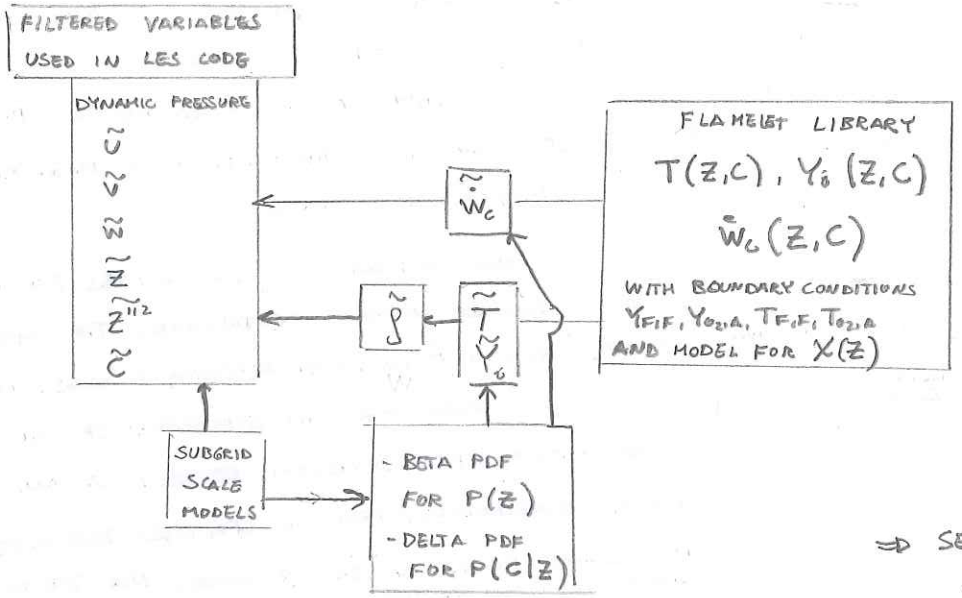
$$\bar{\dot{w}}_C = \int_0^1\int_0^1 \dot{w}_C(Z,C)\,P(Z,C)\,dZ\,dC$$

WHERE THE PROFILES $T(Z,C)$, $Y_i(Z,C)$ AND $\dot{w}_C(Z,C)$ ARE OBTAINED FROM FLAMELET LIBRARIES AND $\tilde{P}(Z,C) = \tilde{P}(C|Z)\,\tilde{P}(Z)$, WITH $\tilde{P}(Z)$ AN ASSUMED BETA SUBGRID PDF (SEE PREVIOUS SECTION) THAT IS FED WITH $\tilde{Z}$ AND $\widetilde{Z''^2}$ → SUBGRID VARIANCE AS PARAMETERS, AND $\tilde{P}(C|Z) = \delta(C - \tilde{C}|_Z)$

A DELTA FUNCTION FOR $\tilde{P}(C|Z)$ IS CHOSEN BY ASSUMING THAT EACH SUBGRID SPACE IS ONLY AFFECTED BY 1 FLAMELET, WITH $\widetilde{C|Z} = C(Z, \Psi_0)$ OBTAINED DIRECTLY FROM THE FLAMELETS AND $\Psi_0$ A PARAMETER WHICH ENSURES THAT $\tilde{C} = \int_0^1 C(Z, \Psi_0)\,\tilde{P}(Z)\,dZ$ IS CONSISTENT WITH THE $\tilde{C}$ RESULTING FROM THE CONSERVATION EQUATION FOR $\tilde{C}$.

ONCE THAT THE FLAMELET LIBRARY HAS BEEN COMPUTED AND THE ASSUMED PDF INTEGRALS HAVE BEEN EVALUATED, LOOKUP TABLES CAN BE GENERATED TO PROVIDE THE FILTERED CHEMICAL VARIABLES AS FUNCTIONS OF THE QUANTITIES READILY AVAILABLE FROM LES ($\tilde{Z}$, $\widetilde{Z''^2}$ AND $\tilde{C}$): THIS IS TYPICALLY OBTAINED FROM ALGEBRAIC MODELS: $\widetilde{Z''^2} = C_g \tilde{\Delta}^2 |\nabla \tilde{Z}|^2$

$$\tilde{Y}_{i_0} = \tilde{Y}_{i_0}(\tilde{Z}, \widetilde{Z''^2}, \tilde{C}), \quad \tilde{T} = \tilde{T}(\tilde{Z}, \widetilde{Z''^2}, \tilde{C}), \quad \tilde{\dot{w}}_C = \tilde{\dot{w}}_C(\tilde{Z}, \widetilde{Z''^2}, \tilde{C})$$




THE FPVA-LES APPROACH

⇒ SEE FIGS 7–9 FOR AN EXAMPLE

FIG 4

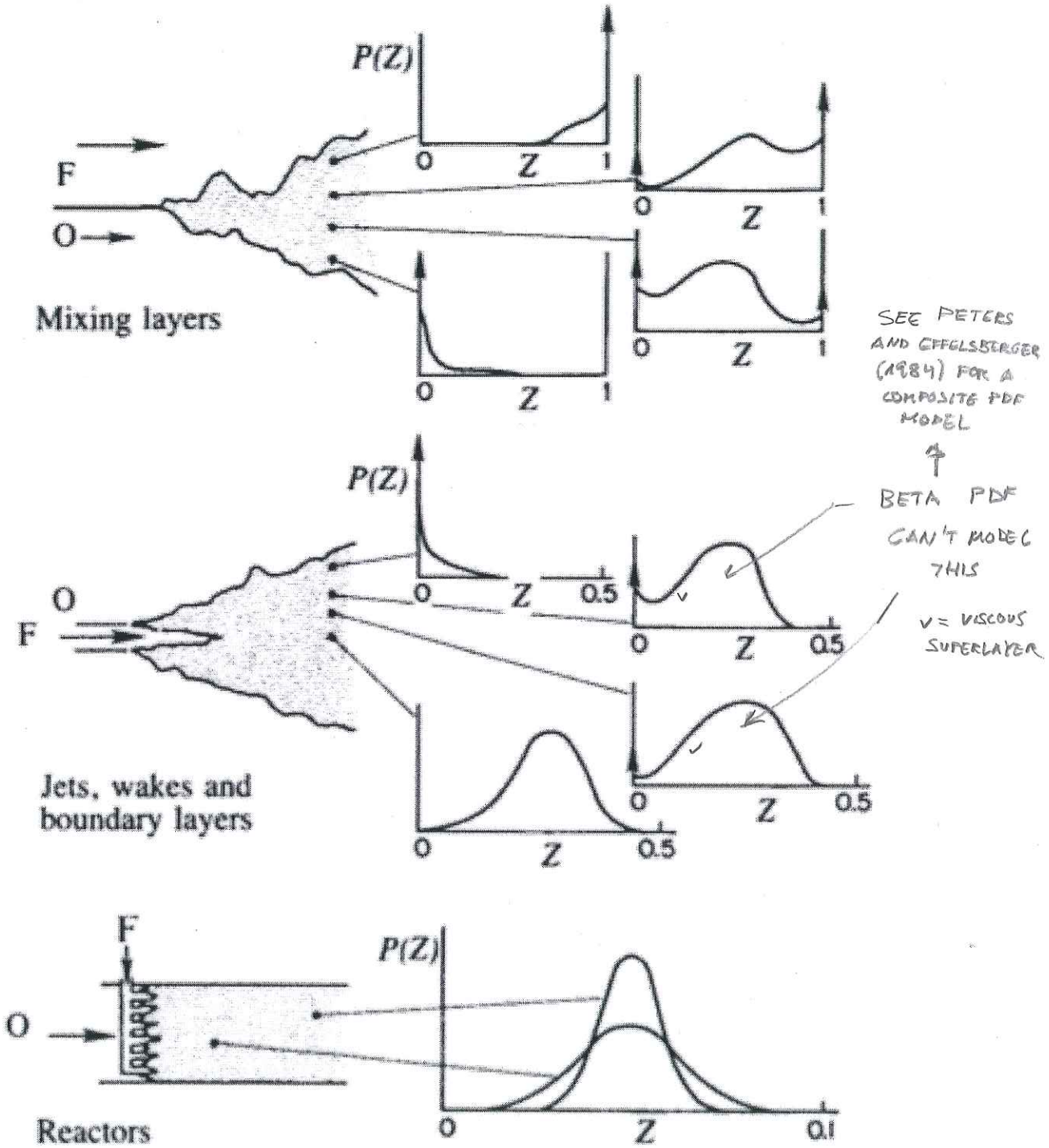
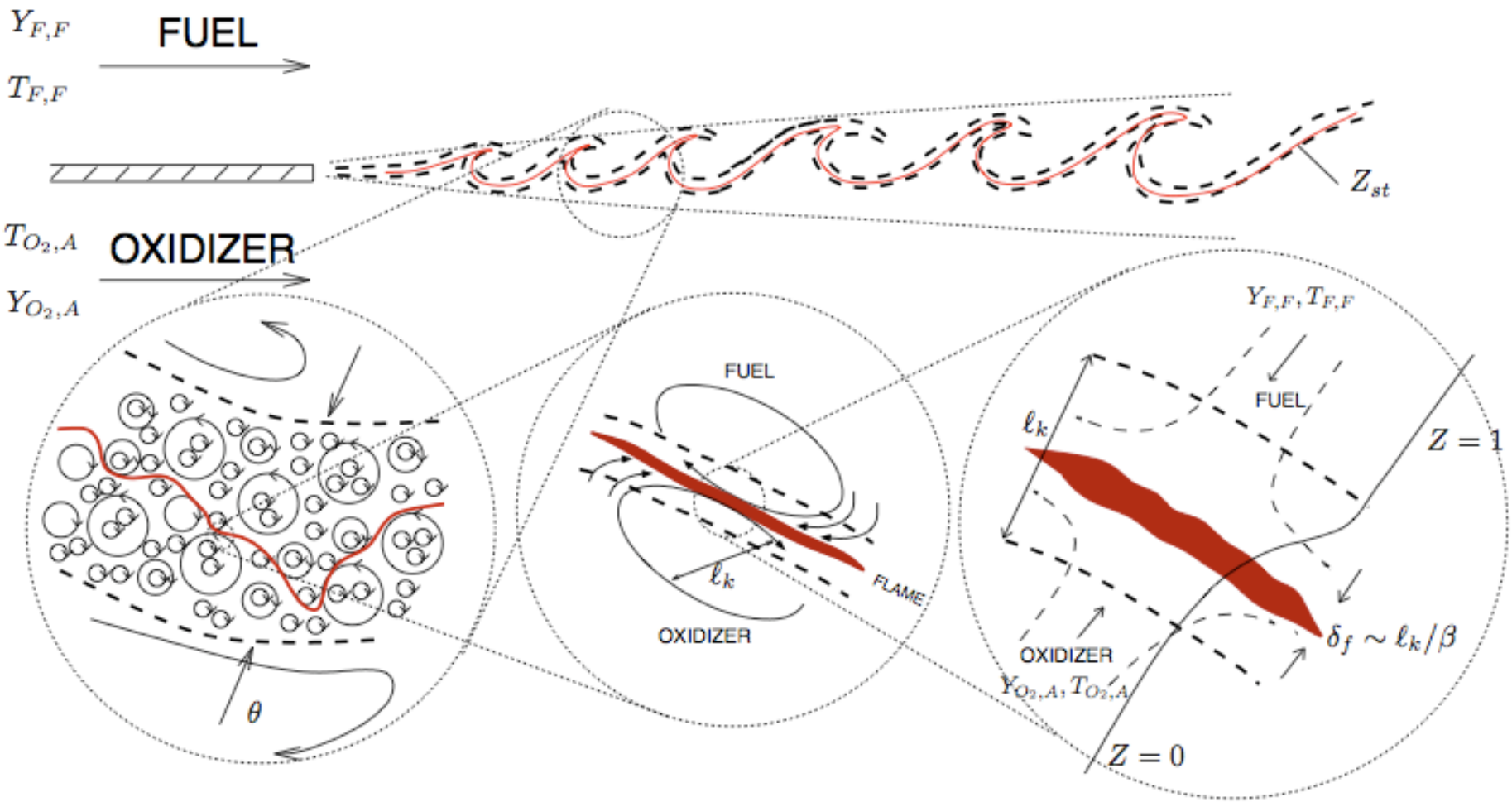



**FIGURE 10.1.** Illustrations of shapes of probability-density functions for the mixture fraction in many turbulent flows (adapted from the contribution of R. W. Bilger to [27]).

# Non-Premixed Turbulent Combustion




THE FLAMELET CONCEPT

STEADY FLAMELETS (EQUILIBRIUM LIMIT)

POINSOT + VEYNANTE (2005)

FIG 5

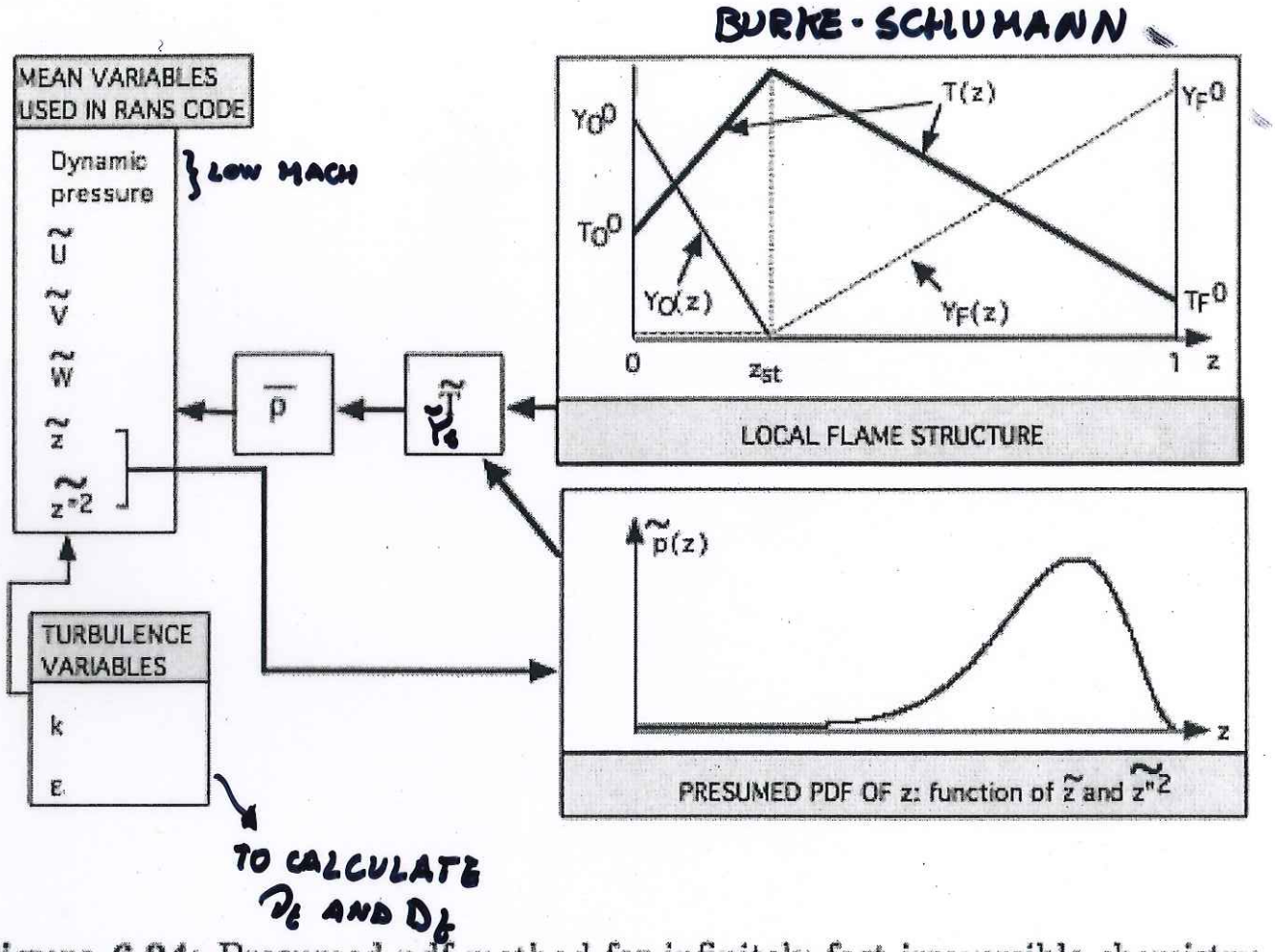



**Figure 6.24:** Presumed pdf method for infinitely fast irreversible chemistry.

POINSOT + VEYNANTE (2005)

FIG 6

# STEADY FLAMELETS (FINITE-RATE CHEMISTRY)

TABULATION OF $Y_k(Z, \chi_{st})$, $T(Z, \chi_{st})$, SOLUTIONS OF $\rho \chi_z \frac{\partial^2 \phi}{\partial Z^2} = -\dot{w}_\phi$ WITH $\phi = Y_k, T$; AND $\begin{cases} \phi = \phi_{F,F} (Z = \\ \phi = \phi_{O_2,A} (Z = 0 \end{cases}$

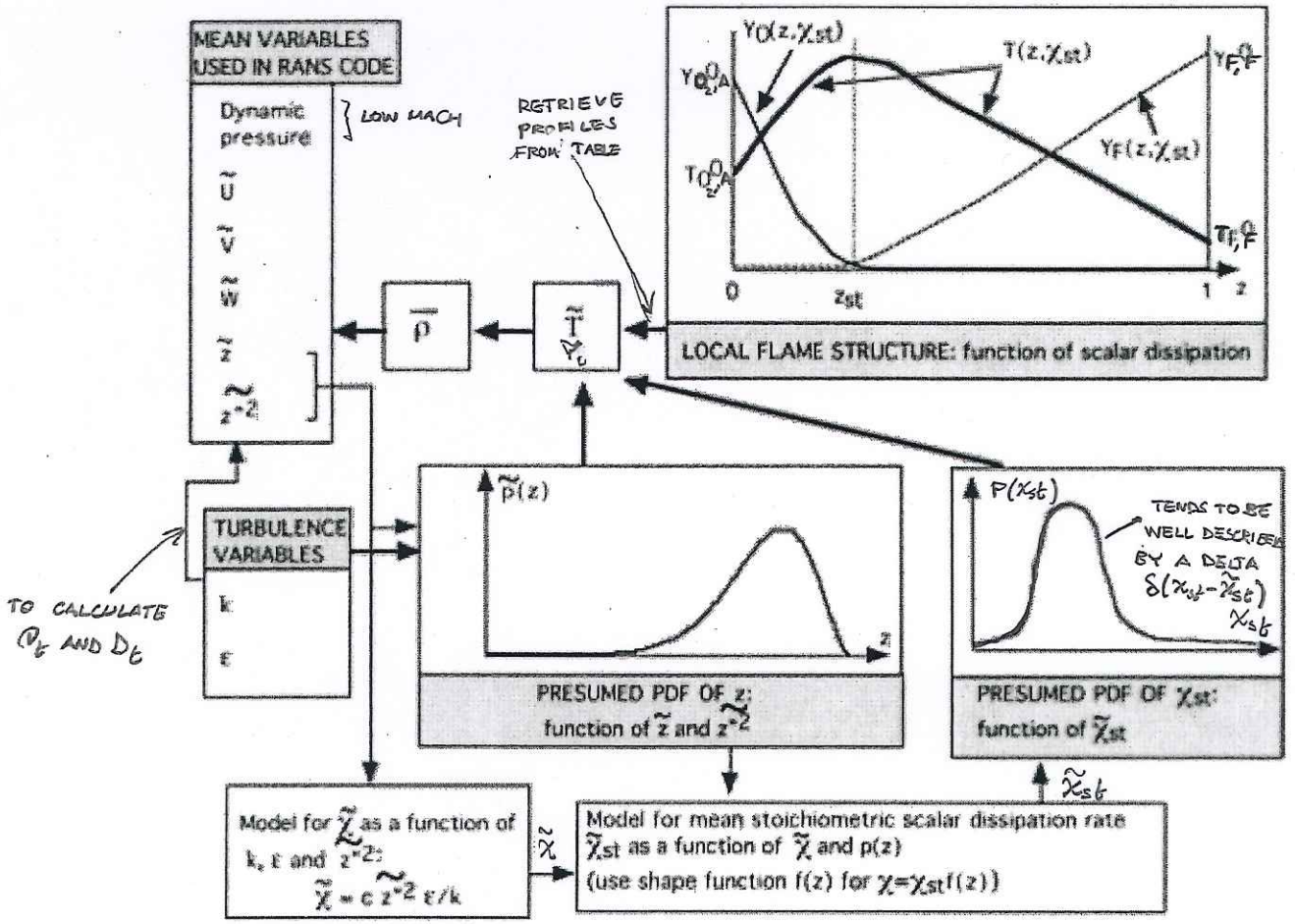
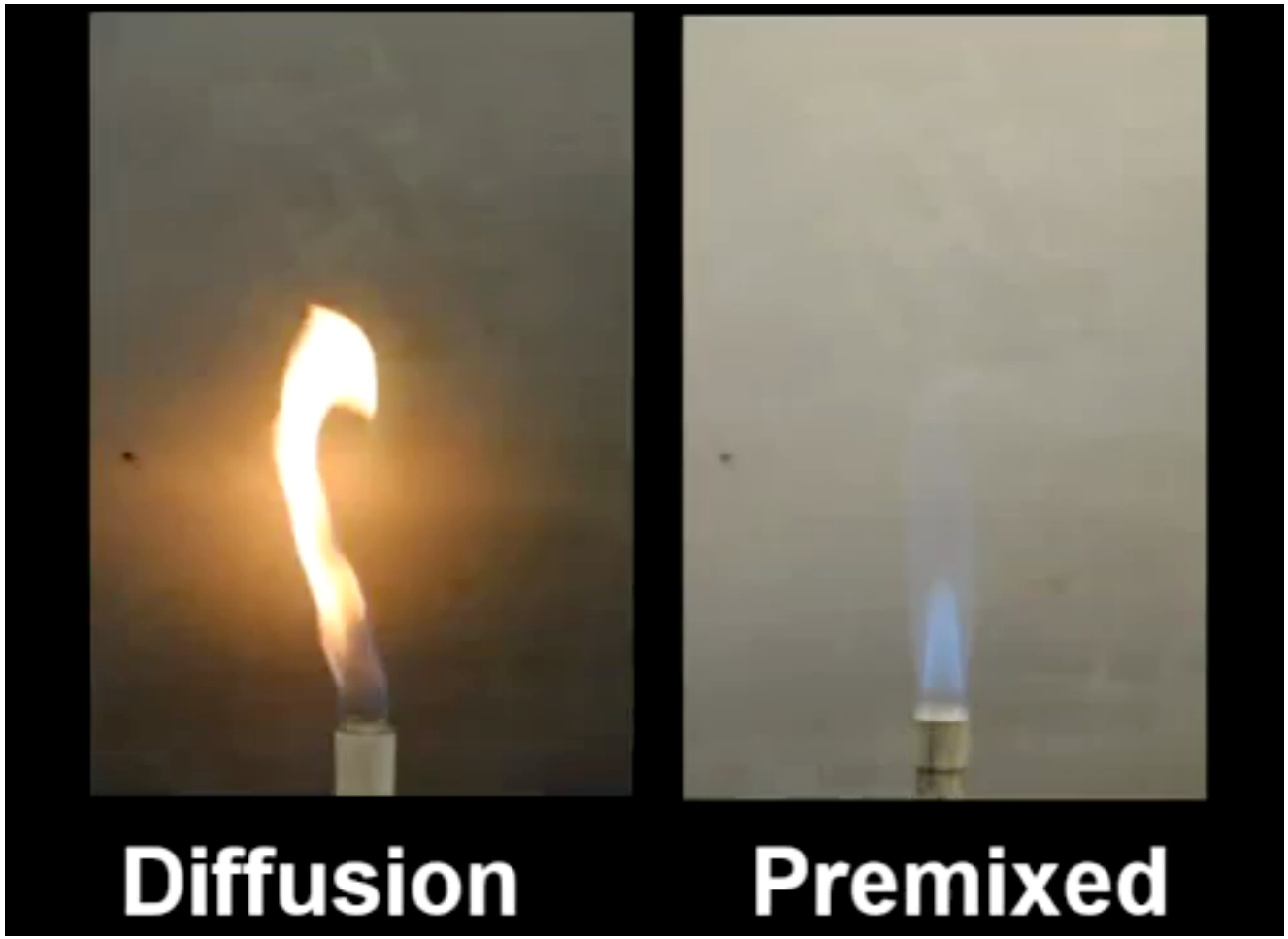



**Figure 6.29:** Organization of a pdf-flamelet model using primitive variables: ~~mean species mass~~

# Non-Premixed Turbulent Combustion



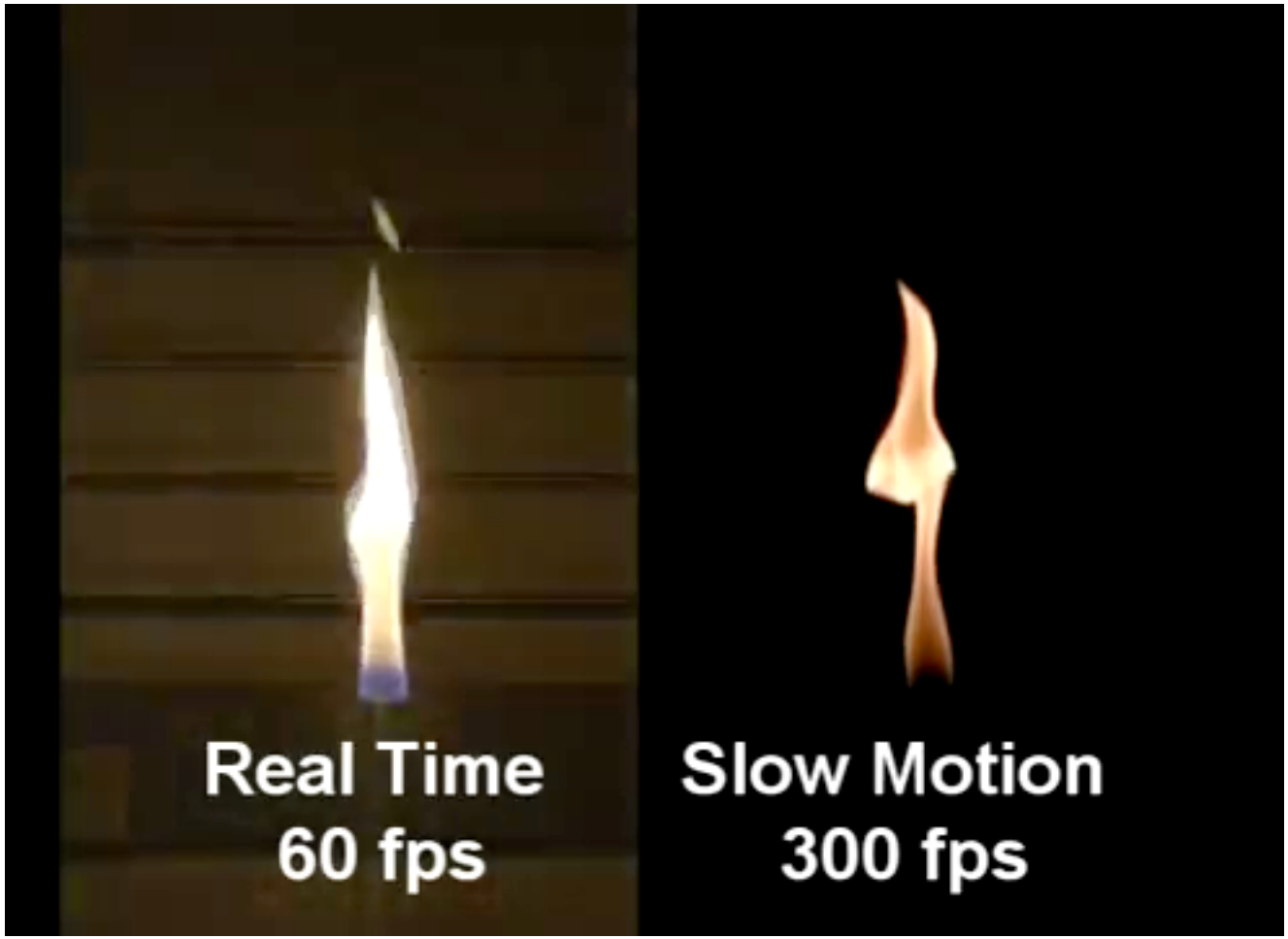

(Movie)

# Non-Premixed Turbulent Combustion




(Movie)

# Non-Premixed Turbulent Combustion



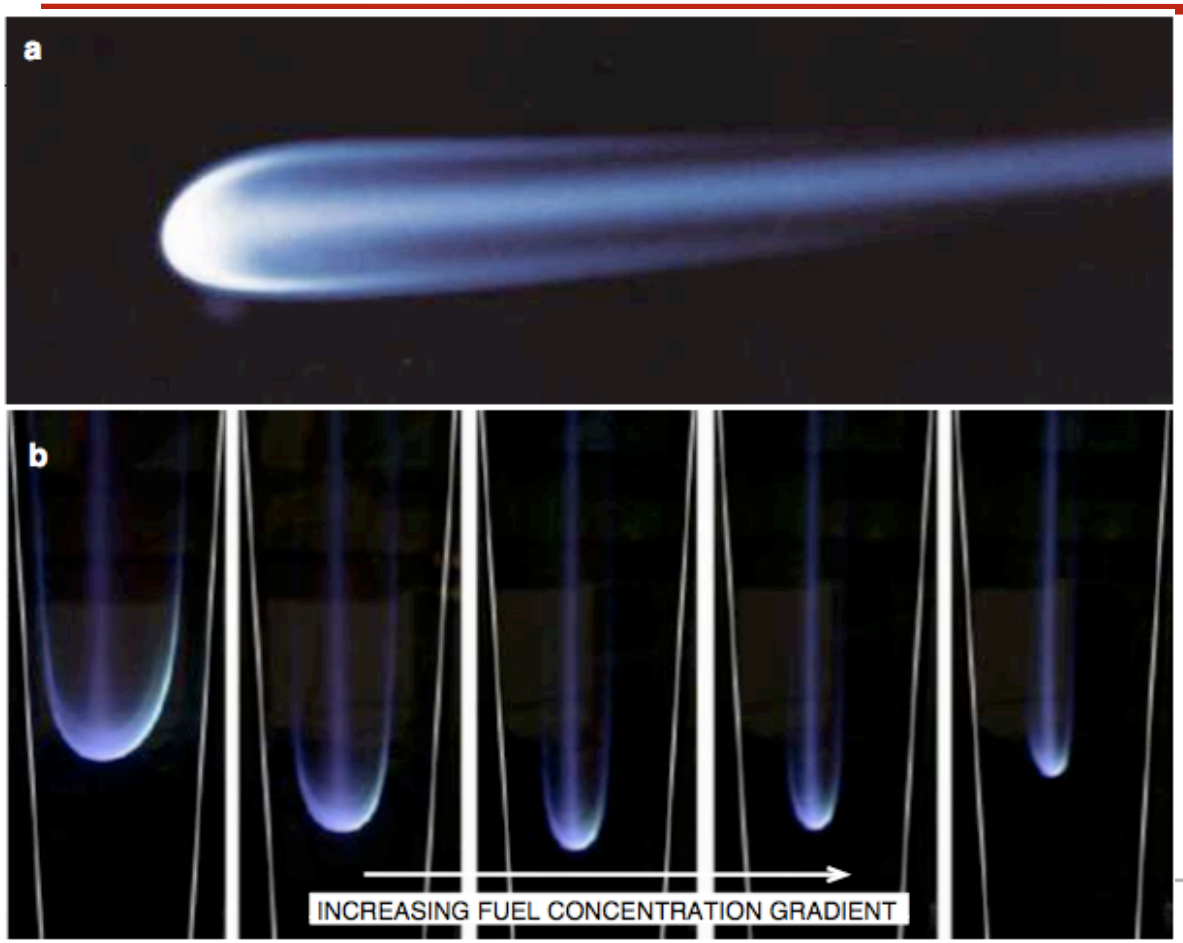

(Movie)

# Non-Premixed Turbulent Combustion

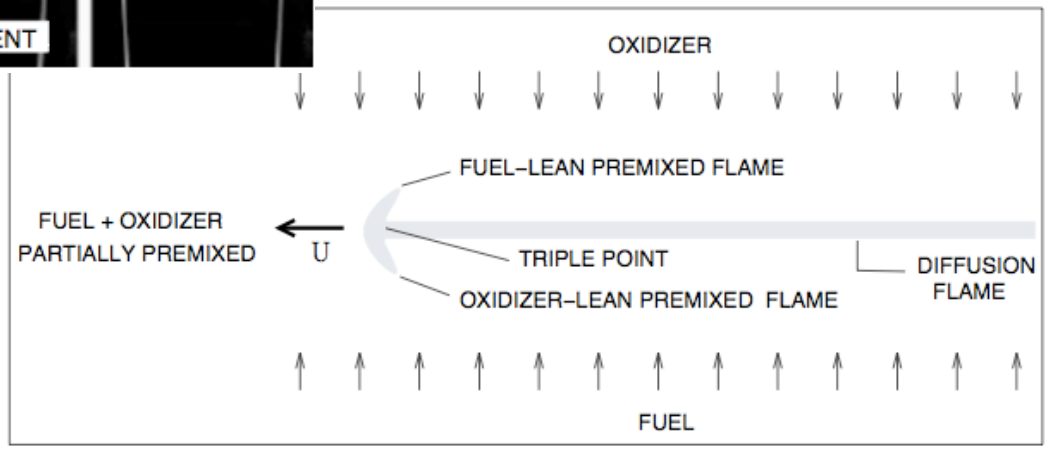


(Movie)

# Non-Premixed Turbulent Combustion




Triple Flames (Kioni et al, 1996)



# Diffusion Flames



(Movie)

# Diffusion Flames

Carlton–Ritz Hotel
(Half-Moon Bay, CA)



(Movie)

# Diffusion Flames

Droplet Combustion (ISS Experiments)



(Movie)

# Non-Premixed Turbulent Combustion

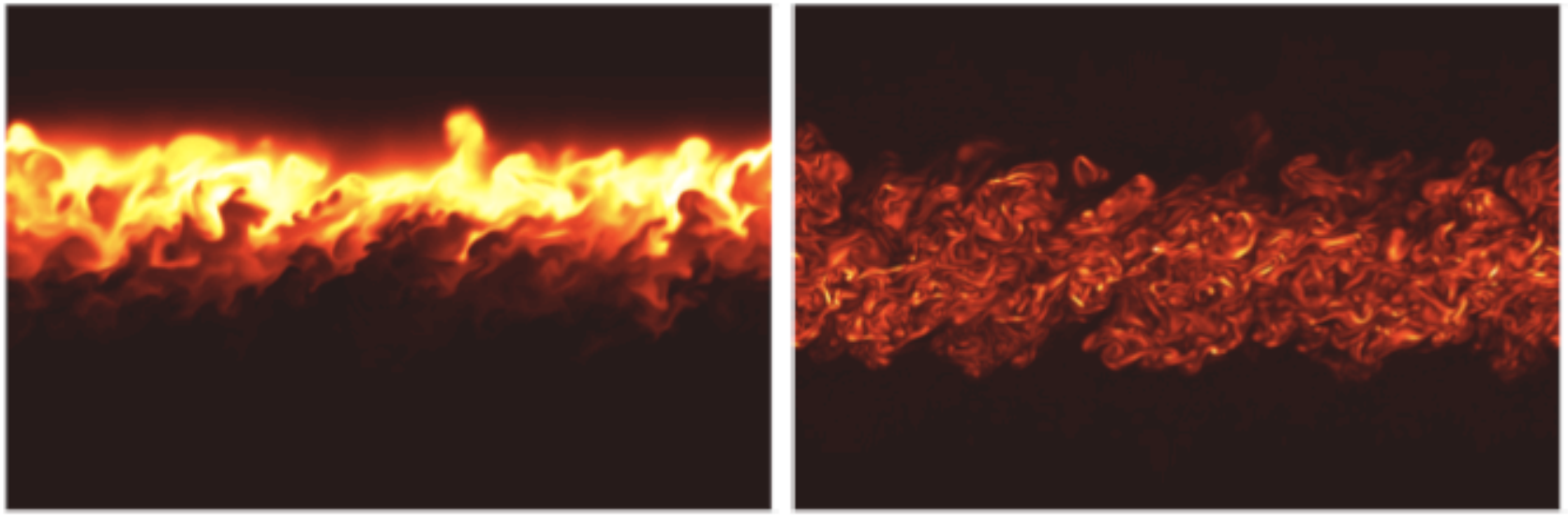


Figure 1: Hydrogen combustion in supersonic time-evolving mixing layer with convective Mach number of 2.5. Instantaneous OH mass fraction (left) and vorticity magnitude (right) in a plane normal to the spanwise direction.

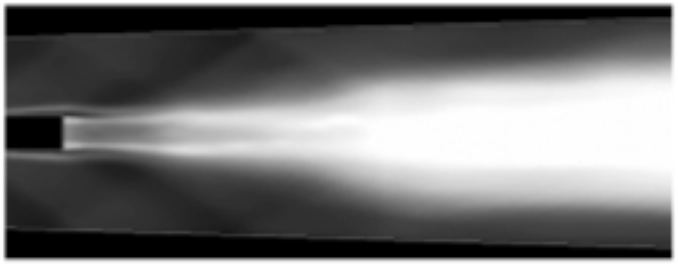
Supersonic mixing layer,
Saghafian and Pitsch (2011)

# Non-Premixed Turbulent Combustion



**Figure 1(b). Fuel injector strut set in the combustor**

LES



d)

Supersonic combustion
Sunami et al., Berglund et al.

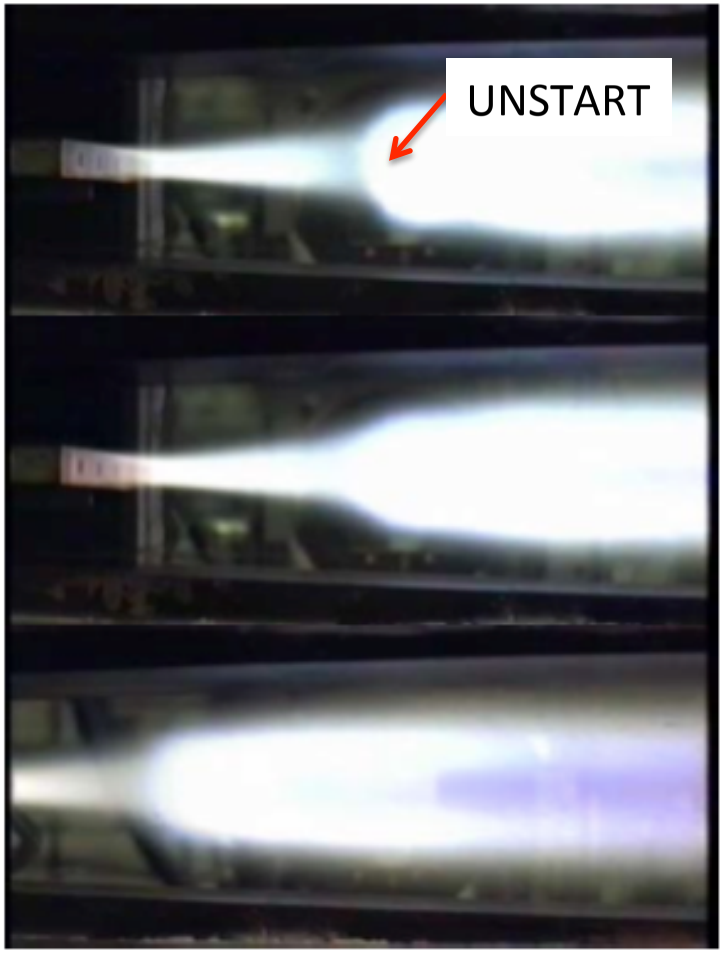
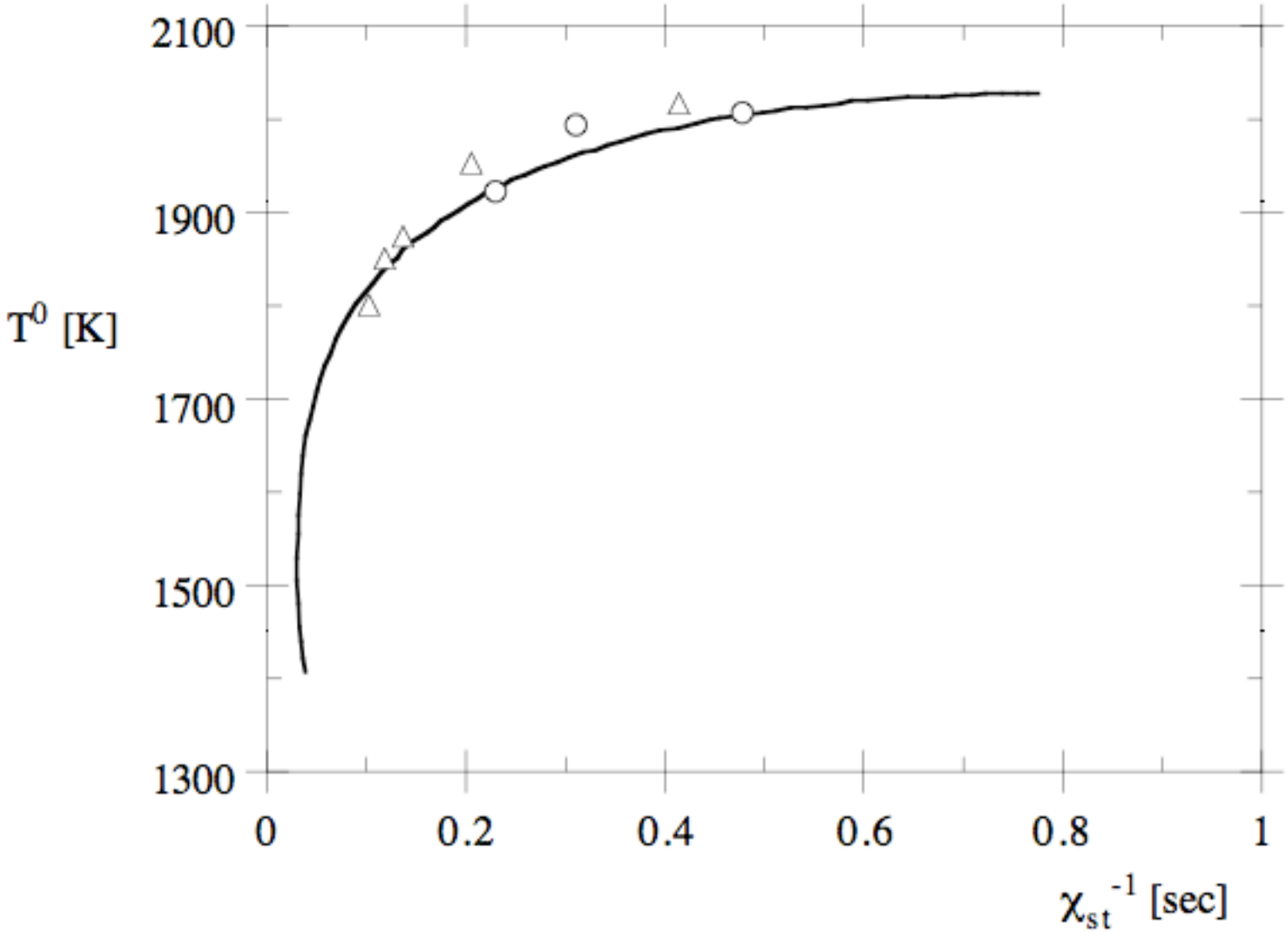



**Figure 9(c). Spontaneous flame images obtained for ONH10 using normal video camera at $\Phi = 0.45$**

# Diffusion Flames




Line: 4-step CH4-O2 mechanism (Seshadri+Peters, 1988).
Symbols: Experiments (Smooke et al. 1986).

# Diffusion Flames

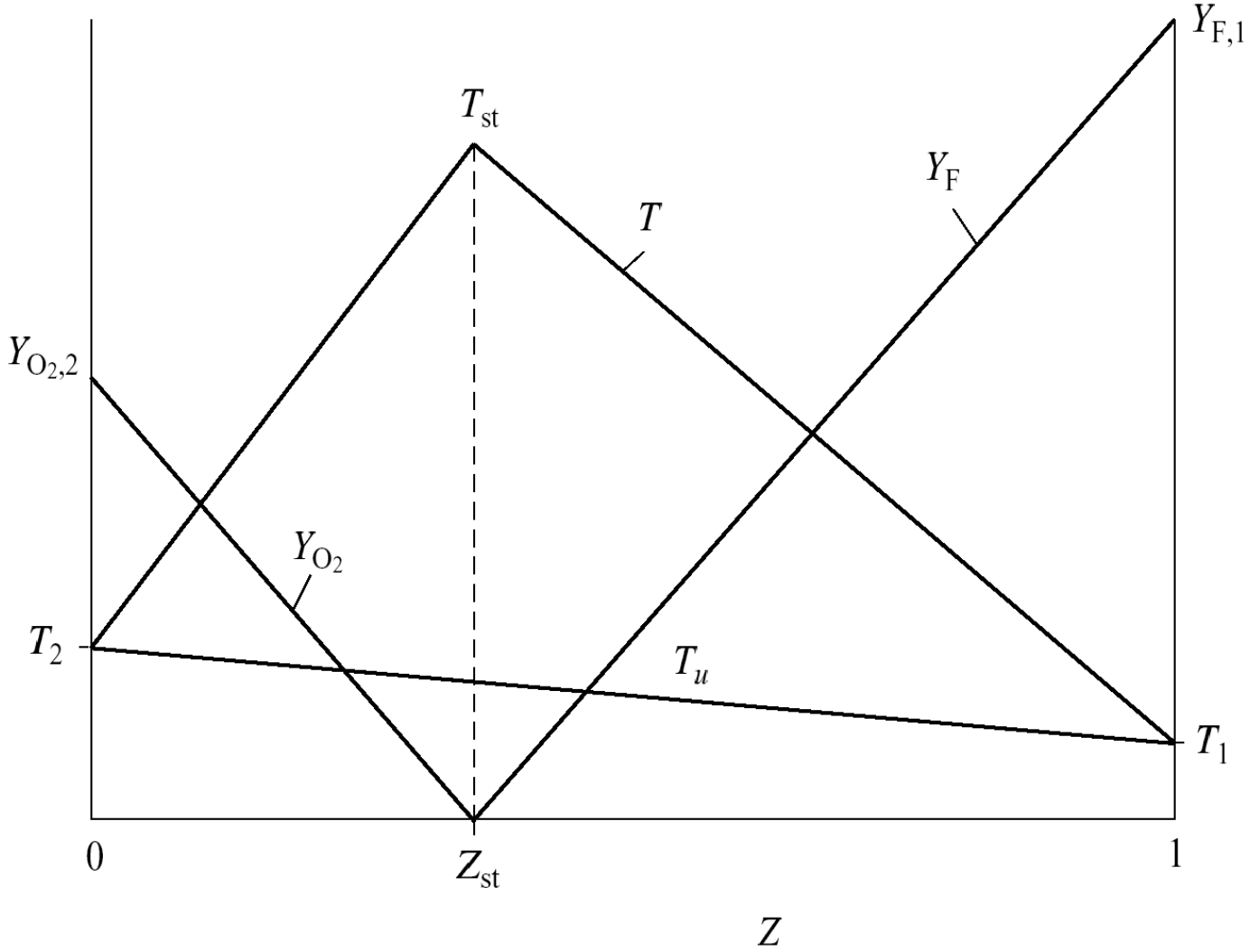



FIG1

BURKE-SCHUMANN LIMIT

# Non-Premixed Turbulent Combustion

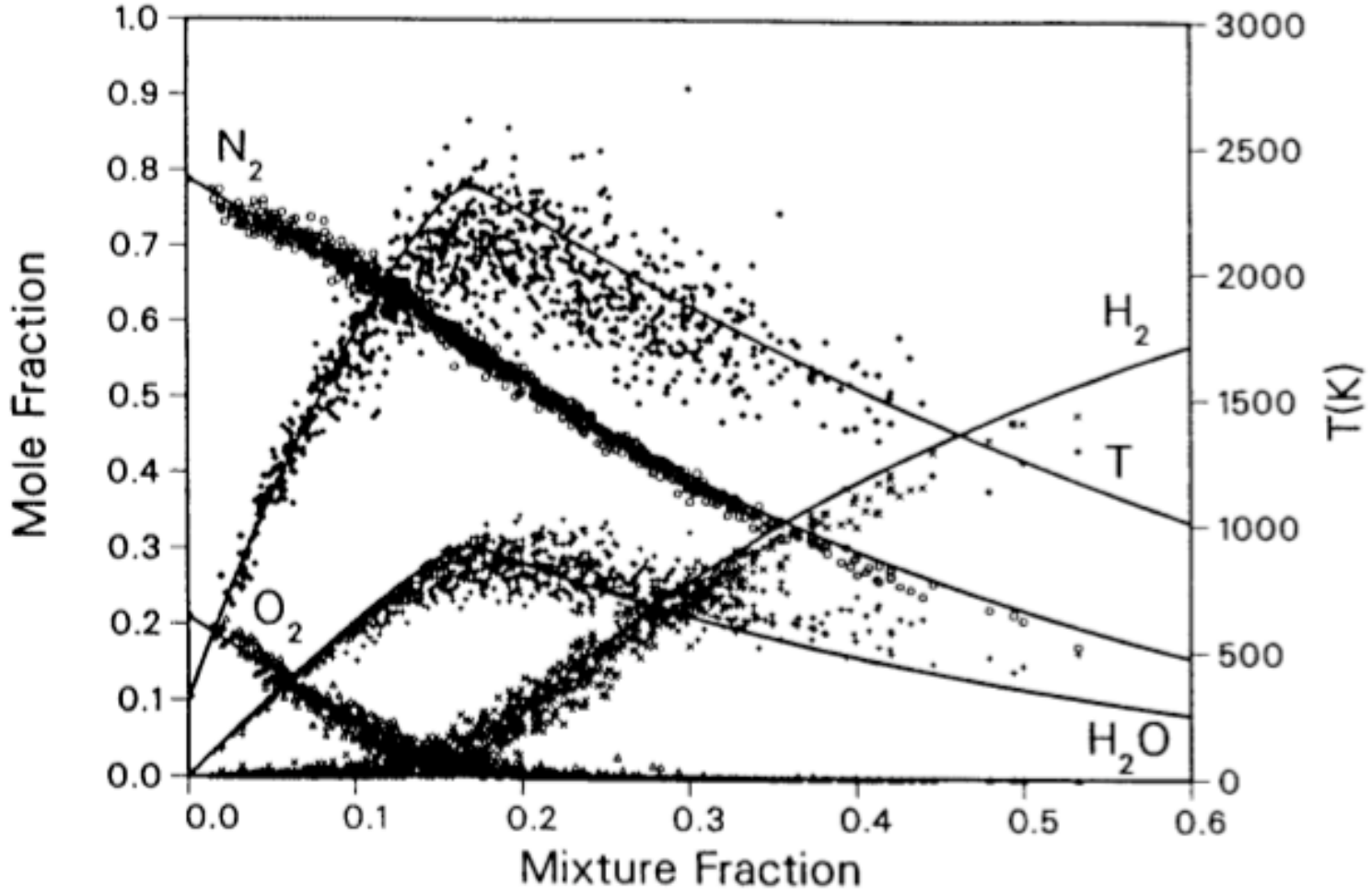



FIG 2

Non-equilibrium effects

Fig. 12.2: Ensemble of Raman scattering measurements of major species concentrations and temperatures at $s/d = 30, r/D = 2$. The solid curves show equilibrium conditions.

# Non-Premixed Turbulent Combustion

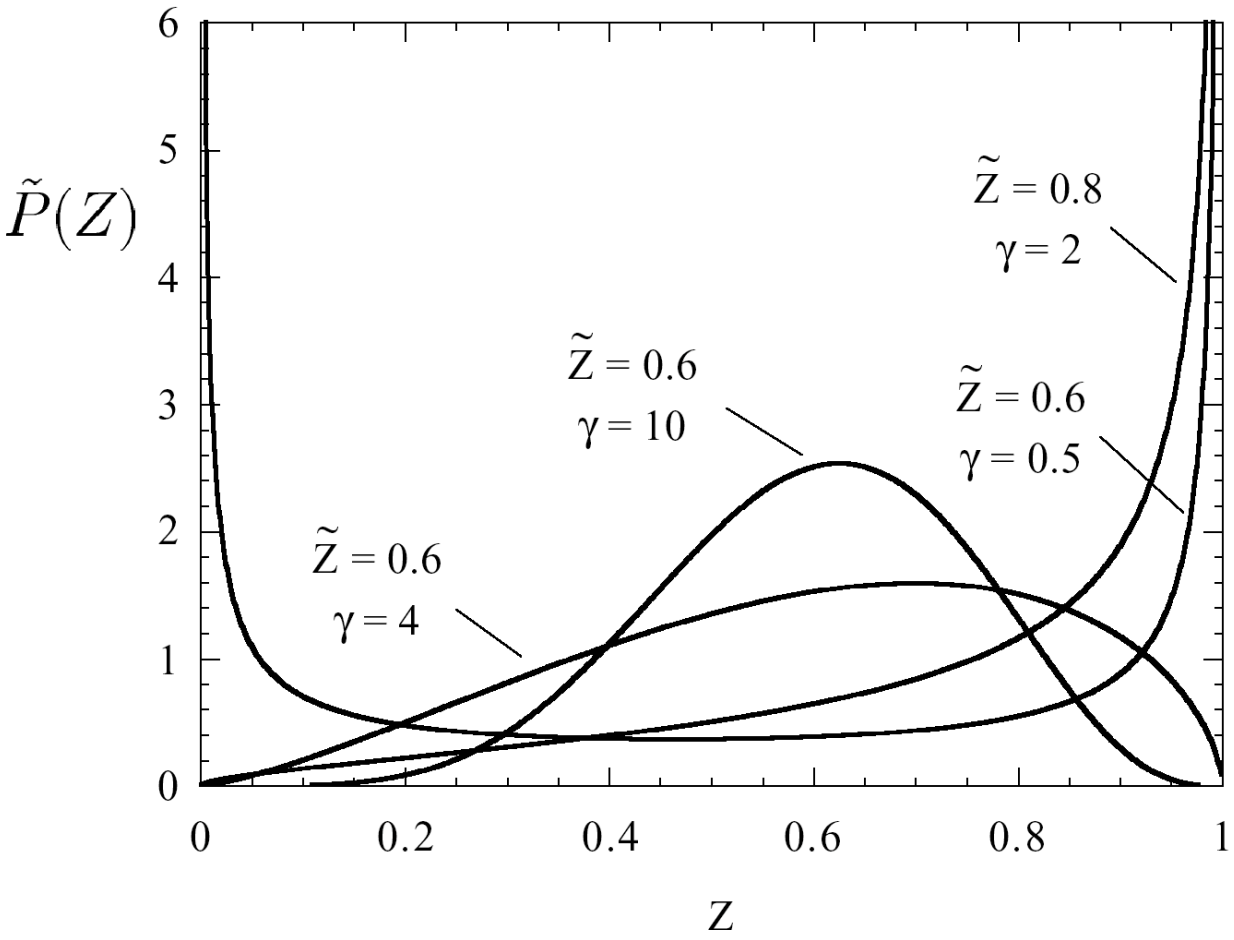



FIG 3

BETA PDF

PIERCE+MOIN (2004)

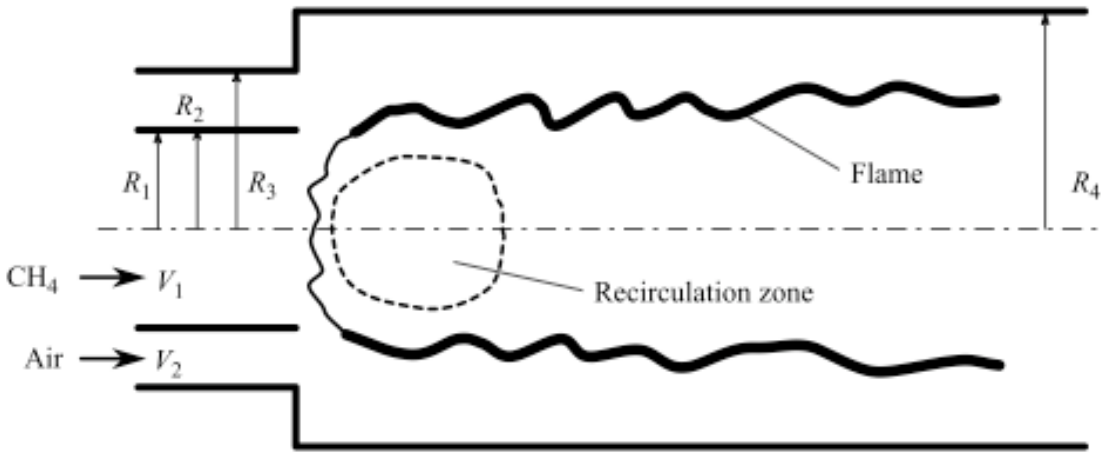



FIGURE 4. Schematic of the coaxial jet combustor experiment.

| | |
|---|---|
| central pipe radius ($R_1$): | 3.157 cm |
| annular inner radius ($R_2$): | 3.175 cm |
| annular wall thickness ($R_2 - R_1$): | 0.018 cm |
| annular outer radius ($R_3$): | 4.685 cm $\equiv R$ |
| combustor radius ($R_4$): | 6.115 cm |
| combustor length: | 100.0 cm |
| mass flow rate of fuel: | 0.00720 kg s$^{-1}$ |
| mass flow rate of air: | 0.137 kg s$^{-1}$ |
| bulk velocity of fuel ($V_1$): | 0.9287 m s$^{-1}$ |
| bulk velocity of air ($V_2$): | 20.63 m s$^{-1}$ $\equiv U$ |
| overall equivalence ratio: | 0.9 |
| temperature of fuel: | 300 K |
| temperature of air: | 750 K |
| combustor pressure: | 3.8 atm |

FIG 7

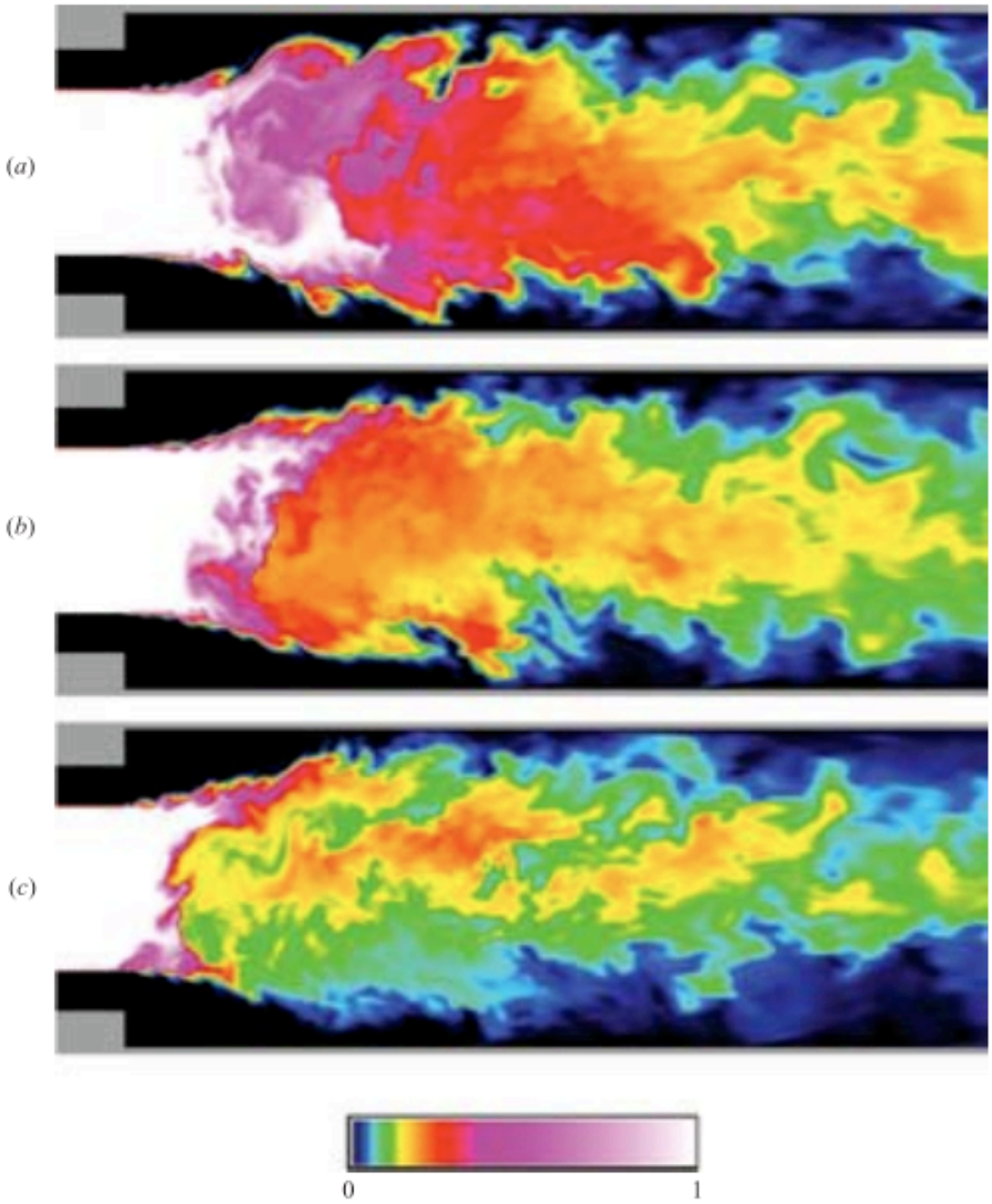



FIGURE 6. Snapshot of mixture fraction in a meridional plane: (*a*) fast-chemistry; (*b*) steady-flamelets; (*c*) progress-variable approach.

FIG 8

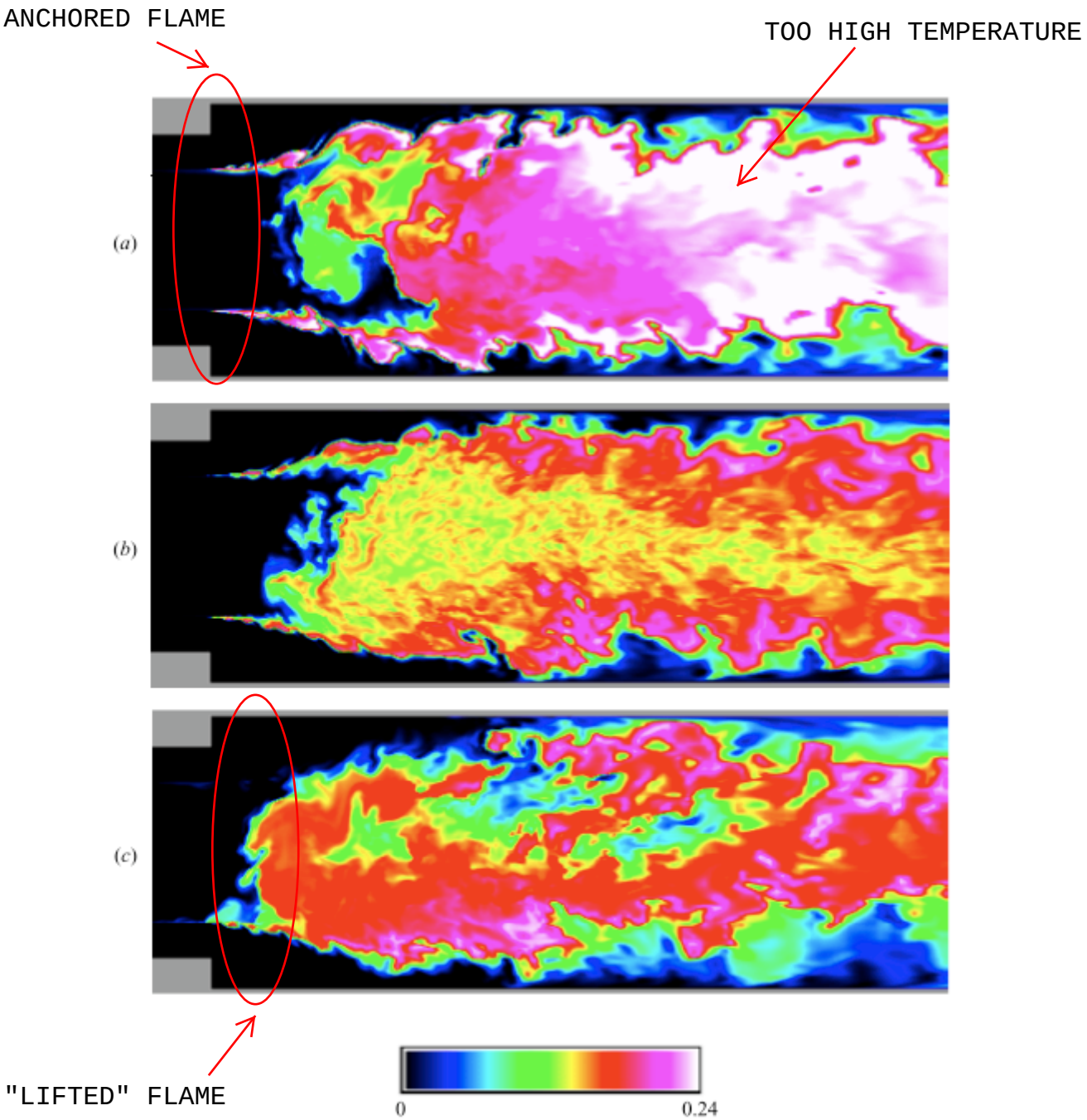



FIGURE 7. Snapshot of product mass fraction in a meridional plane: (*a*) fast-chemistry; (*b*) steady-flamelets; (*c*) progress-variable approach.

PIERCE+MOIN (2004)

FIG 9

C = Y(H20)+Y(CO2)

STANFORD
MECHANICAL
ENGINEERING

**ME 471: TURBULENT COMBUSTION**

**Spring 2012**

# Homeworks

# and

# Exams

J. Urzay

# ME 471: Turbulent Combustion, Spring 2012

**Stanford University**

**Homework 1: Review of combustion and turbulent flows**

Due Tuesday, April 24, in class.

**Guidelines:** Please turn in a *neat* and *clean* homework that gives all the formulae that you have used as well as details that are required for the grader to understand your solution. Show all work. Required plots should be generated using computer software such as Matlab or similar program. Answers should be written in the blank spaces provided in these homework sheets. Use the back of the page in case you need additional space (not recommended to use more space than provided), for which a clear indication should be written to warn the reader of the presence of text there. Vector quantities are denoted in **bold** letters in what follows.

**Student's Name:** JAVIER URZAY ..... **Student's ID:** .....

**Question 1** (20 pts)

The conservation equation for the sensible enthalpy $h_s = \sum_{i=1}^{N} h_{s,i} = \sum_{i=1}^{N} Y_i \int_{T^0}^{T} c_{p,i} dT$ can be written as

$$\rho \frac{\mathrm{D}h_s}{\mathrm{D}t} = \frac{\mathrm{D}P}{\mathrm{D}t} + \tau' : \nabla \mathbf{v} + \nabla \cdot (\kappa \nabla T - \sum_{i=1}^{N} \rho h_{s,i} Y_i \mathbf{V_i}) + \sum_{i=1}^{N} \rho Y_i \mathbf{f_i} \cdot \mathbf{V_i} - \sum_{i=1}^{N} \dot{w}_i h_i^0 + \dot{Q}_r,$$

with $N$ the number of species, $\rho$ the density, $\mathbf{v}$ the velocity, $P$ the pressure, $\tau'$ the viscous stress tensor, $\kappa$ the thermal conductivity and $\dot{Q}_r$ the radiated heat. Similarly, $Y_i$ is the mass fraction, $\mathbf{V_i}$ is the diffusion velocity, $\mathbf{f_i}$ is the body force, $\dot{w}_i$ is the mass production rate, $h_i^0$ is the formation enthalpy and $c_{p,i}$ is the specific heat at constant pressure of species $i$.

**a)** From this equation, derive a conservation equation for the temperature $T$ in terms of the material derivative $\mathrm{D}T/\mathrm{D}t$.

SINCE $\rho \frac{Dh_s}{Dt} = \sum_{i=1}^{N} \rho \frac{DY_i}{Dt} \int_{T^0}^{T} c_{p_i} dT + \sum_{i=1}^{N} \rho Y_i c_{p_i} \frac{DT}{Dt} = \sum_{i=1}^{N} \dot{w}_i \int_{T^0}^{T} c_{p_i} dT - \sum_{i=1}^{N} \nabla \cdot (\rho \underline{V_i} Y_i) \int_{T^0}^{T} c_{p_i} dT$

$+ \sum_{i=1}^{N} \rho c_p \frac{DT}{Dt}$, THEN THE CONSERVATION EQUATION FOR THE SENSIBLE ENTHALPY BECOMES:

$\rho c_p \frac{DT}{Dt} = \frac{DP}{Dt} + \bar{\bar{\tau}}' : \nabla \underline{v} + \nabla \cdot (\kappa \nabla T) - \sum_{i=1}^{N} \rho \underline{V_i} Y_i c_{p_i} \nabla T + \sum_{i=1}^{N} \rho Y_i \underline{f_i} \cdot \underline{V_i} + \dot{Q}_R - \sum_{i=1}^{N} (h_i^0 + \int_{T^0}^{T} c_{p_i} dT) \dot{w}_i$

WITH $c_p = \sum_{i=1}^{N} Y_i c_{p_i}$ THE AVERAGE SPECIFIC HEAT

+25

**b)** Simplify the conservation equation obtained in part a) for the case in which the following conditions are satisfied simultaneously: i) the Mach number is small, ii) all species have equal $c_{p,i}$, iii) the radiation heat is negligible, iv) the background pressure is steady, v) and the body forces are negligible.

AT LOW MACH: $\frac{\bar{\bar{\tau}}' : \nabla v}{\rho c_p \underline{v} \cdot \nabla T} \sim O\left(\frac{M^2}{Re}\right) \ll 1$, WITH $M \sim U/c$ AND $Re = UL/\nu$

IF $c_{p_i} = c_p$, THEN $\sum_{i=1}^{N} \rho \underline{V_i} Y_i c_{p_i} \nabla T = \rho c_p \nabla T \sum_{i=1}^{N} \underline{V_i} Y_i = 0$ AND $\sum_{i=1}^{N} h_i \dot{w}_i = \sum_{i=1}^{N} h_i^0 \dot{w}_i + \int_{0}^{T} c_p dT \sum_{i=1}^{N} \dot{w}_i$

IF $P \neq P(t) \Rightarrow DP/Dt = 0$

THEN $\rho c_p \frac{DT}{Dt} = \nabla \cdot (\kappa \nabla T) - \sum_{i=1}^{N} h_i^0 \dot{w}_i$

+25

**Student's Name:** JAVIER URZAY

**Question 2** (50 pts).

Asymptotic expansions of the Boltzmann equation indicate that the diffusion velocities $\mathbf{V_i}$ of species $i$ in a multicomponent mixture of $N$ species can be calculated from the equation

$$\nabla X_i = \sum_{j=1}^{N} \left(\frac{X_i X_j}{D_{ij}}\right)(\mathbf{V_j} - \mathbf{V_i}) + (Y_i - X_i)\left(\frac{\nabla P}{P}\right) + \frac{\rho}{P}\sum_{j=1}^{N} Y_i Y_j(\mathbf{f_i} - \mathbf{f_j}) + \sum_{j=1}^{N}\left(\frac{X_i X_j}{\rho D_{ij}}\right)\left(\frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i}\right)\left(\frac{\nabla T}{T}\right)$$

(see for instance, "Molecular theory of gases and liquids" by Hirschfelder, Curtiss and Bird, 1964) where $\rho$ is the density, $P$ is the pressure, $T$ is the temperature, $X_i$ is the molar fraction of species $i$, $Y_i$ is the mass fraction of species $i$, $D_{ij}$ is the binary diffusion coefficient and $D_{T,i}$ is the Soret coefficient of species $i$.

**a)** Give a qualitative description of the four different terms; in what conditions are each of them negligible?

+5 ①: CONCENTRATION GRADIENTS GENERATED BY DIFFERENT DIFFUSION VELOCITIES → MAIN EFFECT

+5 ②: " " " BY PRESSURE GRADIENTS AND DIFFERENT MOLECULAR WEIGHTS
↳ BARODIFFUSION, NEGLIGIBLE WHEN $\nabla P/P \ll 1$ OR $W_i = \overline{W}$

+5 ③ " " " BY DIFFERENT BODY FORCES ACTING ON DIFFERENT SPECIES
↳ NEGLIGIBLE WHEN $f_i = f_1$

+5 ④: " " " BY TEMPERATURE GRADIENTS. NEGLIGIBLE WHEN $\frac{\nabla T}{T} \ll 1$ OR $\frac{D_{T,i}}{\rho D_{ij}} \ll 1$

**b)** Show that this equation reduces to the Fick's law $\mathbf{V_i} Y_i = -D_{ij}\nabla Y_i$ if all the following conditions are satisfied simultaneously: i) the mixture is binary, ii) the thermal diffusion is negligible, iii) the pressure gradients are small compared to the pressure itself, and iv) the body forces acting on each species are equal.

+20

WHEN i) + ii) + iii) ARE SATISFIED: $\nabla X_i = \sum_{j=1}^{N}\left(\frac{X_i X_j}{D_{ij}}\right)(\underline{V_j} - \underline{V_i})$ (1)

FOR BINARY MIXTURES: $Y_1 + Y_2 = 1$, $X_1 + X_2 = 1$.

WITH $X_1 = \frac{Y_1 \overline{W}}{W_1}$ AND $X_2 = \frac{Y_2 \overline{W}}{W_2}$ ⇒ $\nabla X_1 = \frac{\overline{W}}{W_1}\nabla Y_1 + Y_1 \frac{\nabla \overline{W}}{W_1}$, SUBSTITUTING

THIS RESULT ON (1),

$$\frac{\overline{W}\nabla Y_1}{W_1} + \frac{Y_1}{W_1}\nabla \overline{W} = \frac{Y_1 Y_2}{D_{12}}(\underline{V_2} - \underline{V_1})\frac{\overline{W}^2}{W_1 W_2}$$

AND SINCE $W_1 Y_1 + W_2 Y_2 = 0$, THEN $-\frac{\underline{V_1} Y_1}{D_{12}} = \left(\frac{Y_1 W_2}{W_1} + (1 - Y_1)\right)\nabla Y_1 - Y_1 W_2 \nabla\left(\frac{1}{W}\right)$

$$= \frac{Y_1 W_2}{W_1}\nabla Y_1 + \nabla Y_1 - Y_1 \nabla Y_1 - \frac{Y_1 W_2}{W_1}\nabla Y_1 + Y_1 \nabla Y_1$$

AND

$$\Rightarrow \underline{V_1} Y_1 = -D_{12}\nabla Y_1$$ +10

**Student's Name:** JAVIER URZAY

**Problem 1** (50 pts)

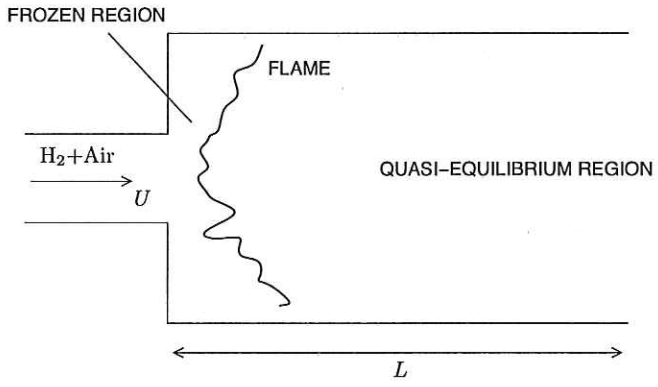
In the design of turbulent-combustion chambers for gas turbines, a careful consideration of pollutant emissions is of particular importance for compliance with current regulations.

Consider a combustion chamber in which a lean mixture of hydrogen $H_2$ and air is burnt to generate high enthalpy gases that will be sent to the turbine stage. The mixture is injected at a temperature $T_u = 298$ K and the chamber operates at atmospheric pressure. In this combustor, all the NO is produced by the Zel'dovich mechanism, which is given by the set of chemical reactions

$$N_2 + O \rightarrow NO + N \quad (1)$$
$$N + O_2 \rightarrow NO + O \quad (2)$$
$$N + OH \rightarrow NO + H \quad (3)$$
$$O_2 \rightleftharpoons 2O \quad (4)$$

The Zel'dovich mechanism (1)-(4) describes the production of NO by the high-temperature dissociation of the $N_2$ found in the air premixed with the $H_2$. Other NO production mechanisms - such as the Fenimore mechanism for prompt NO formation by hydrocarbon radical action upon $N_2$, or mechanisms of NO formation from fuel-bound nitrogen - are irrelevant here since the fuel is pure hydrogen.

A strongly corrugated premixed flame is produced as a result of the chemical reactions and the turbulence in the combustor, as depicted in Fig. 1. The flame front separates an entrance region, in which the temperature is low and the chemistry is frozen, from a quasi-equilibrium region, in which the temperature is high and all species concentrations (except NO) reach the values given by chemical equilibrium. The production of NO occurs mainly in this second region because of the slow rate of the NO chemistry and its strong dependence on temperature. To illustrate the influences of the equivalence ratio, consider three different gaseous mixtures at the injection: i) Mixture A with $Y_{H_2,u} = 0.015$ balanced with air, and ii) Mixture B with $Y_{H_2,u} = 0.025$ balanced with air.




0.5/EACH

**a)** Obtain the composition of the fresh gases ($Y_{N_2,u}$, $X_{N_2,u}$, $Y_{O_2,u}$, $X_{O_2,u}$, $Y_{H_2,u}$, $X_{H_2,u}$ and equivalence ratio $\phi$) for the two initial mixtures A and B.

+1/0/0

MIXTURE A): $Y_{H_2U} = 0.015 = 1 - Y_{N_2U} - Y_{O_2U}$ (+0.5) AND SINCE IN AIR: $\frac{X_{O_2}}{X_{N_2}} = \frac{1}{3.76} = 0.26 = \frac{Y_{O_2} W_{N_2}}{Y_{N_2} W_{O_2}} \rightarrow \frac{Y_{O_2}}{Y_{N_2}} = 0.304$

THEN $Y_{N_2U} = \frac{1 - Y_{H_2U}}{1.304} = 0.755$, AND $Y_{O_2U} = 0.2296$. +0.5 +0.5

ALSO, $\overline{W_u} = \frac{1}{\frac{Y_{H_2U}}{W_{H_2}} + \frac{Y_{O_2U}}{W_{O_2}} + \frac{Y_{N_2U}}{W_{N_2}}} = 24.01$ g/mol $\Rightarrow$

$X_{H_2U} = \frac{Y_{H_2U}\overline{W_u}}{W_{H_2}} = 0.18$ +0.5

$X_{O_2U} = \frac{Y_{O_2U}\overline{W_u}}{W_{O_2}} = 0.172$ +0.5

$X_{N_2U} = \frac{Y_{N_2U}\overline{W_u}}{W_{N_2}} = 0.647$ +0.5

ALSO, $\phi = \frac{X_{H_2U}/X_{O_2U}}{2} = 0.52$ +0.5

MIXTURE B): REPEATING THE SAME PROCEDURE: +0.5 +0.5

$Y_{H_2U} = 0.025$, $Y_{N_2U} = 0.747$, $Y_{O_2U} = 0.227$, $X_{H_2U} = 0.27$, $X_{O_2U} = 0.175$, $X_{N_2U} = 0.576$, $\phi = 0.77$ +0.5 +0.5 +0.5 +0.5 +0.5 +0.5

7/7

**Student's Name:**

**b)** Assuming that the burnt gases only contain $N_2$, $O_2$ and $H_2O$ (i.e. the concentration of other species are much smaller), use the conservation of atoms to determine the molar fractions and mass fractions of the products in the quasi-equilibrium zone for the fresh mixtures A and B.

GLOBAL REACTION: $H_2 + N_{O_2U}(O_2 + 3.76N_2) \rightarrow H_2O + N_{O_2b}O_2 + 3.76N_{O_2U}N_2$ ± 0.5/EACH

- FOR MIXTURE A): $N_{O_2U} = 1/2\phi = 0.96$ MOLES/MOL $H_2$

CONS ATOMS: H: $2 = N_{H_2O_b} \cdot 2 \rightarrow N_{H_2O_b} = 1$ MOL/MOL $H_2$

O: $0.96 \cdot 2 = 2N_{O_2b} + N_{H_2O} \rightarrow N_{O_2b} = 0.46$ MOL/MOL $H_2$

N: $3.76\,N_{O_2U} = N_{N_2b} = 3.61$ MOLES/MOL $H_2$

TOTAL MOLES IN PRODUCTS: $N_{H_2O_b} + N_{O_2b} + N_{N_2b} = 5.07 = N_T$

$X_{O_2b} = \frac{N_{O_2b}}{N_T} = 0.09$

$X_{N_2b} = \frac{N_{N_2b}}{N_T} = 0.71$

$X_{H_2O_b} = \frac{N_{H_2Ob}}{N_T} = 0.197$

$Y_{O_2b} = 0.109$

$Y_{N_2b} = 0.755$

$Y_{H_2O_b} = 0.135$

- FOR MIXTURE B): $Y_{O_2b} = 0.027$, $Y_{H_2b} = 0.225$, $Y_{N_2b} = 0.7477$, $X_{O_2b} = 0.0213$

$X_{H_2Ob} = 0.312$, $X_{N_2b} = 0.666$

**c)** Calculate the adiabatic temperature in the quasi-equilibrium region for the fresh mixtures A and B. To simplify the calculations, assume that the specific heat of the mixture is $c_p = 1.4$ kJ/kgK for both fresh and burnt gases.

THE ADIABATIC FLAME TEMPERATURE IS GIVEN BY THE CONSERVATION OF TOTAL ENTHALPY:

$$\sum_{i=1}^{N} Y_i h_i\Big|_{\text{REACTANTS}} = \sum_{i=1}^{N} Y_i h_i\Big|_{\text{PRODUCTS}} \rightarrow \text{WITH } h_i = h_i^o + \int_{T^o}^{T} c_{pi}\,dT \quad (h^o_{N_2} = h^o_{O_2} = h^o_{H_2} = 0)$$

THEN $Y_{O_2U}\cancel{h^o_{O_2}} + Y_{H_2U}\cancel{h^o_{H_2}} + Y_{N_2U}\cancel{h^o_{N_2}} + c_p T_U = Y_{O_2b}\cancel{h^o_{O_2}} + Y_{N_2b}\cancel{h^o_{N_2}} + Y_{H_2O_b}h^o_{H_2O} + c_p T_b$

SO THAT $T_b = T_U - \frac{Y_{H_2O_b} h^o_{H_2O}}{c_p}$, WITH $h^o_{H_2O} = -13.4 \cdot 10^3$ kJ/kg

- FOR MIXTURE A): $T_b = 1590$ K +5
- FOR MIXTURE B): $T_b = 2451$ K +5

10/10

**d)** In order to obtain the production rate of NO, use the Zel'dovich mechanism given in the problem statement and follow these steps (show the work):

$[\dot{N}] = 0$

i) Assume that the N radical is in steady state, or equivalently, that the rates of the steps 2 and 3 are much faster than the rate of step 1. In this way, you should be able to write down an equation for the production rate $\dot{\omega}_{NO}$ that only depends on the concentrations of $N_2$ and O.

$[\dot{N}] = \dot{\omega}_1 - \dot{\omega}_2 - \dot{\omega}_3 = 0 \rightarrow \dot{\omega}_1 = \dot{\omega}_2 + \dot{\omega}_3$ WITH $\dot{\omega}_1 = k_1[N_2][O]$, $\dot{\omega}_2 = k_2[N][O_2]$, $\dot{\omega}_3 = k_3[N][OH]$

$[\dot{NO}] = \dot{\omega}_1 + \dot{\omega}_2 + \dot{\omega}_3 = 2\dot{\omega}_1 = 2k_1[N_2][O] = \dot{\omega}_{NO}$

5/5

ii) Assume that step 4 is in chemical equilibrium, and obtain a relation between the concentrations of O and $O_2$ in equilibrium.

IF $O_2 \overset{4}{\rightleftharpoons} 2O$ IS IN CHEMICAL EQUILIBRIUM, THE EQUILIBRIUM CONSTANT BECOMES

$$K_{C4} = \frac{[O]^2_{eq}}{[O_2]_{eq}} \rightarrow [O]_{eq} = K_{C4}^{1/2}[O_2]_{eq}$$

5/5

$$\Rightarrow \dot{\omega}_{NO} = 2k_1 K_{C4}^{1/2} [O_2]_{eq} [N_2]$$

**Student's Name:**

After performing successfully steps i) and ii), you would obtain

$$\frac{d[\mathrm{NO}]}{dt} = \dot{\omega}_{\mathrm{NO}} = k[\mathrm{N_2}][\mathrm{O_2}]_{eq}^{1/2} \tag{5}$$

where $k = 2k_1 K_{c4}^{1/2}$, where $k_1$ is the rate constant of reaction (1) and $K_{c4}$ is the concentration equilibrium constant of reaction (4). You can use this result if you were not able to obtain it using i) and ii) above.

e) Using equation (5), estimate the molar fraction of NO at the combustor exit for the fresh mixtures A and B if the characteristic injection velocity of the fresh gases is $U = 10$ m/s and the combustor length is $L = 10$ cm. Notice that $\tau \sim L/U$ is a characteristic integral length of the problem that can be used in (5) to estimate $X_{\mathrm{NO}}$. For solving this part, assume $k = 1.83 \cdot 10^{15} \left(\frac{\mathrm{cm}^3}{\mathrm{s^2 mol}}\right)^{1/2} \exp\left[-\frac{567.5\mathrm{kJ/mol}}{R^0 T}\right]$.

$X_{NO} = \frac{[NO]}{[M]}$, $[M] = \frac{P}{RT}$

$\frac{d[NO]}{dt} = [M]\frac{dX_{NO}}{dt} = k[M]^{3/2} X_{N_2} X_{O_2 eq}^{1/2} \Rightarrow \frac{dX_{NO}}{dt} = k X_{N_2 b} X_{O_2 b}^{1/2} \left(\frac{P}{R^0 T_{ad}}\right)^{1/2}$

THEN $X_{NO} \sim k X_{N_2 b} X_{O_2 b}^{1/2} \left(\frac{P}{R^0 T_{ad}}\right)^{1/2} \tau$ WITH $\tau \sim L/U = 10\,ms$

- FOR MIXTURE A): $X_{N_2 b} = 0.71$, $X_{O_2 b} = 0.09$, $T_{ad} = 1590k$ $\Rightarrow$ $k = 4.06 \cdot 10^{7} \left(\frac{m^3}{s^2 mol}\right)^{1/2}$ $\Rightarrow X_{NO} \sim 2.39 \cdot 10^{-9}$ +4.25

$X_{NO}$ INCREASES A LOT WITH $\phi$!

- FOR MIXTURE B): $X_{N_2 b} = 0.666$, $X_{O_2 b} = 0.0213$, $T_{ad} = 2451\,k$ $\Rightarrow$ $k = 1.46 \left(\frac{m^3}{s^2 mol}\right)^{1/2}$ $\Rightarrow X_{NO} \sim 3165\ ppm = 3.165 \cdot 10^{-6}$ +4.25

8.5/8.5

f) If the combustion chamber was sufficiently long, then the residence time in the quasi-equilibrium region would be large and the concentration of NO would reach the equilibrium value. This concentration can be obtained by assuming that the reaction

$$\mathrm{N_2 + O_2 \rightleftharpoons NO + NO} \tag{6}$$

is in chemical equilibrium. Use the results from part b) and the chemical-equilibrium constraint on reaction (6) to obtain the molar fraction of NO at the combustor exit for mixtures A and B, and compare it to the results obtained from e). The comparison should indicate that chemical equilibrium ~~always~~ TENDS TO overestimates the production of NO in typical combustors.

AT EQUILIBRIUM: $K_P = e^{-\frac{2 g^0_{NO}}{R^0 T_{ad}}} = \frac{X_{NO}^2}{X_{N_2 b} X_{O_2 b}}$, WITH $g^0_{NO} = 70.15\ \frac{kJ}{mol}$ AT 1600 k

$g^0_{NO} = 58.71\ kJ/mol$ AT 2500 k

- FOR MIXTURE A): $K_P = 2.48 \cdot 10^{-5}$, $X_{NO} = 1262$ ppm +4.25
- FOR MIXTURE B): $K_P = 3.25 \cdot 10^{-3}$, $X_{NO} = 0.00679$ +4.25

LARGER THAN WITHOUT EQUILIBRIUM.

8.5/8.5

# ME 471: Turbulent Combustion, Spring 2012

**Stanford University**

**Homework 2: Review of turbulent flows (II) and Premixed Turbulent Combustion (I)**

Due Tuesday, May 8 in class.

**Guidelines:** Please turn in a *neat* and *clean* homework that gives all the formulae that you have used as well as details that are required for the grader to understand your solution. Show all work. Required plots should be generated using computer software such as Matlab or similar program. Answers should be written in the blank spaces provided in these homework sheets. Use the back of the page in case you need additional space (not recommended to use more space than provided), for which a clear indication should be written to warn the reader of the presence of text there. Vector quantities are denoted in **bold** letters in what follows.

**Student's Name:** JAVIER URZAY **Student's ID:**

**Solve either Question 1 or Question 2, and solve Problem 1.**

**Question 1** (50 pts)

**a)** Obtain a relation between the Favre average $\widetilde{\phi}$ and the Reynolds average $\overline{\phi}$ for a scalar field $\phi = \phi(\mathbf{x}, t)$. Why is Favre averaging used in formulations of turbulent combustion?

FAVRE: $\phi = \widetilde{\phi} + \phi''$ SUCH THAT $\overline{\phi'' \rho} = 0$ } THEN $\overline{\rho\phi} = \overline{\rho(\widetilde{\phi} + \phi'')} = \overline{\rho}\widetilde{\phi}$, AND ALSO

REYNOLDS: $\phi = \overline{\phi} + \phi'$ $\overline{\rho\phi} = \overline{\rho(\overline{\phi} + \phi')} = \overline{\rho}\overline{\phi} + \overline{\rho'\phi'} \Rightarrow \boxed{\overline{\rho}\widetilde{\phi} = \overline{\rho}\overline{\phi} + \overline{\rho'\phi'}}$ +10

⇒ THERE ISN'T A SIMPLE RELATION BETWEEN FAVRE AVERAGES AND REYNOLDS AVERAGES. THE CORRELATION $\overline{\rho'\phi'}$ IS REQUIRED TO TRANSFORM ONE INTO THE OTHER. FAVRE AVERAGES ARE USED BECAUSE THEY CAN ABSORB THE $\overline{\rho'\phi'}$ TERM THAT OTHERWISE WOULD APPEAR IN THE REYNOLDS AVERAGED CONTINUITY EQ. +10

**b)** Derive a transport equation for the scalar variance $\widetilde{\phi''^2}$. To do this, follow these steps: First derive a transport equation for $\widetilde{\phi^2}$, and then obtain another transport equation for $\left(\widetilde{\phi}\right)^2$. Then use the relation $\widetilde{\phi''^2} = \widetilde{\phi^2} - \left(\widetilde{\phi}\right)^2$ to obtain the transport equation for the scalar variance (use back of the page for more space). Also, give a brief description of each of the different terms in your equation.

SEE PAGE 13 OF INSTRUCTOR'S NOTES FOR DERIVATION +30

**Student's Name:** JAVIER URZAY

**Question 2** (50 pts)

Select true (T) or false (F) for each of the statements in the list provided for each question. A complementary and *brief* mathematical proof / sketch of your answer on the back of the page would be welcome, but it is **not** needed in order to get full credit.

(X INDICATE CORRECT CHOICE)

**2.1** In turbulent flows at high Reynolds numbers,

a) the maximum kinetic energy is located within the Kolmogorov range (T/F)

b) the viscous dissipation generated by the motion of the large eddies is much larger than the turbulent dissipation (T/F)

c) the large scales have turnover times which are much faster than the turnover time of the Kolmogorov eddies (T/F)

d) large-eddy simulations resolve all scales in the flow up to a maximum wave number beyond which physical subgrid-scale models may (or may not) be employed (T/F).

**2.2** In a turbulent flow carrying a scalar $\phi$ with a single integral length scale $\ell = \ell_\phi$, characteristic large-eddy turnover velocity $u'$, molecular diffusivity $D$, and Schmidt number $\mathrm{Sc} = \nu/D$,

a) molecular diffusion of the scalar takes place at the integral scale $\ell$; this is why the turbulent diffusivity $D_t$ is usually defined by relations of the type $u'\ell/D_t = O(1)$ (T/F)

b) there is no molecular diffusion in turbulent flows because in the asymptotic limit of infinite Reynolds numbers $u'\ell/D \to \infty$ the Euler equations are recovered; this is why computing turbulent reacting flows becomes so much more straightforward than computing laminar reacting flows (T/F)

c) molecular diffusion of the scalar $\phi$ takes place at scales of the same order as the Batchelor scale, $\ell_B = \mathrm{Sc}^{-1/2}\ell_k$, where $\ell_k$ is the Kolmogorov scale (T/F)

d) the Reynolds number based on the turbulent diffusivity $D_t$, (i.e. $u'\ell/D_t$) is typically much larger than the Reynolds number based on the molecular diffusivity $D$, (i.e. $u'\ell/D$) (T/F).

**2.3** In the mixing of two reactants in a turbulent flow,

a) the scalar dissipation rate is always a sink in the scalar variance equation (T/F)

b) the scalar dissipation rate indicates zones where molecular mixing is taking place (T/F)

c) the scalar dissipation rate is maximum in zones where only one of the reactants exists (T/F)

d) the scalar dissipation of interest for turbulent combustion is defined as the Reynolds-average of the turbulent diffusivity multiplied by the square of the gradient of the scalar fluctuations (neglecting density variations) (T/F)

e) for order-unity Schmidt numbers, the molecular mixing of two reactants typically occurs in time scales which are much faster than the integral time scale (T/F)

f) macroscopic mixing or stirring is sufficient for having chemical reaction between both reactants (T/F).

+ 50/14 EACH

**Student's Name:**

**Problem 1** (50 pts)

A cylindrical premixed burner in a power plant is designed to burn a stoichiometric mixture of gaseous methane ($CH_4$) and air in a chamber pressurized at 20 bar. A sketch of the burner is shown below. Just upstream of the combustor intake, the $CH_4$–air feed stream has been passed through a grid to promote turbulence, in such a way that a streamwise turbulent intensity 15% and an approximate integral length scale 3 cm are obtained. a) Give an estimate of the resolution requirements required for the direct numerical simulation of this burner in terms of the total number of grid points $N$, the MAX ~~minimum~~ grid spacing $\Delta x$ (make the assumptions that you most like regarding grid topology), the MAX ~~minimum~~ time step $\Delta t$ and the total number of time steps $N_t$ (assume an explicit fully-compressible code). b) Based on the premixed turbulent-combustion diagram explained in class, characterize the combustion regime in which this burner is likely to be operating. (Note: In case you need additional data, you can use external references but make sure you cite them below)

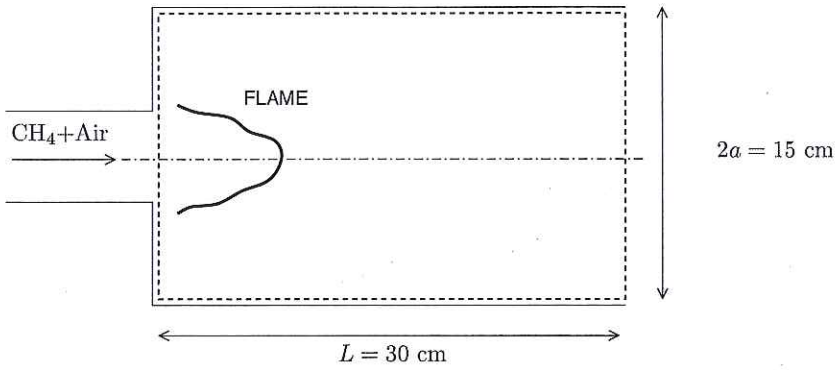



Figure 1: Sketch of the burner. In this figure, $2a$ denotes the diameter of the burner and $L$ its axial length. The dashed line represents the boundaries of the computational domain.

THE INFLOW MEAN VELOCITY $\bar{U}$ NEEDS TO BE OF THE SAME ORDER AS THE PREMIXED FLAME VELOCITY $S_L^0$ FOR STABILIZING THE FLAME (UP TO A MULTIPLICATIVE FACTOR OF ORDER UNITY THAT INDICATES FLOW INHOMOGENEITIES AND AN INCLINATION ANGLE). FOR ESTIMATION PURPOSES, $\bar{U} \sim S_L^0 \sim 15\ cm/s$ (SEE LIÑÁN AND WILLIAMS, 1993 PAGE 54). THEN $0.15 = u'/\bar{U} \rightarrow u' = 2.2\ cm/s$. SINCE $\ell = 0.03\ m$, THEN $Re_\ell = \frac{u'\ell}{\nu} \sim 900$ WITH $\nu \sim \nu_{PATH}^{AIR}/20 \sim 7.5 \cdot 10^{-2}\ m^2/s$. SIMILARLY, $\delta_L^0 \sim Dt/S_L^0 \sim \nu/S_L^0 \sim 10\ \mu m$. NOTE SMALL THICKNESS DUE TO ELEVATED PRESSURE

IN THIS PROBLEM, THE SIZE OF THE KOLMOGOROV EDDIES IS OF ORDER $\ell_K \sim \ell\, Re_\ell^{-3/4} \sim 0.18\ mm$

THE EXTENT OF THE COMPUTATIONAL DOMAIN IS ALREADY LARGE ENOUGH TO CAPTURE THE INFLOW INTEGRAL LENGTH SCALE. HOWEVER, SINCE $\ell_K > \delta_L^0$, THE MAXIMUM $\Delta x$ IS SET BY THE FLAME THICKNESS,

$\delta_L^0 \sim \Delta x\, N_f \sim 10\,\Delta x \rightarrow \Delta x \sim \delta_L^0/10 \sim 1\ \mu m$ +10. THE TOTAL NUMBER OF GRID POINTS IS

$N = N_r N_\theta N_x \sim \frac{L}{\Delta x}\cdot\frac{a}{\Delta x}\cdot N_\theta \sim 10^{15}$ POINTS +10 (WOULD BE EVEN LARGER IF $N_f \sim 100 \Rightarrow$ TOO LARGE COMBUSTOR FOR DNS!)

THE MAXIMUM CHEMICAL TIME STEP REQUIRED MAY BE ESTIMATED AS $\Delta t_c \sim \delta^2 \frac{\delta_L^{0^2}}{\nu} \sim 10^{-6}\ s$, WITH $\delta \sim 0.1$ THE DIMENSIONLESS THICKNESS OF THE FUEL-CONSUMPTION LAYER. THE MAXIMUM TIME STEP BASED ON ACOUSTIC CONSIDERATIONS IS OF ORDER $\Delta t_{US} \sim \Delta x/c \sim 10^{-8}\ s$, WITH $c \sim 340\ m/s$ THE SPEED OF SOUND WAVES. THEN, $\Delta t = \min(\Delta t_{US}, \Delta t_c) = 10^{-8}\ s$ +10. THE MINIMUM NUMBER OF TIME STEPS REQUIRED IS $N_t \sim L/U\Delta t \sim 10^8$ +10 FOR A 1 FLOW-THROUGH TIME. SINCE $u'/S_L < 1$ AND $\delta_L^0 < \ell_K$, THE BURNER IS OPERATING IN THE WRINKLED FLAMELETS +10

# ME 471: Turbulent Combustion, Spring 2012

**Stanford University**

**Midterm Exam**

Tuesday, May 15.

**Closed books, closed notes, no calculator allowed**

**Guidelines:** Please turn in a *neat* and *clean* exam solution. Answers should be written in the blank spaces provided in these exam sheets. Vector quantities are denoted in **bold** letters in what follows.

**Student's Name:** JAVIER URZAY ..... **Student's ID:** .....

**Question 1** (50 pts)

a) Explain the concept of "separation of scales" (Peters, 2000) in turbulent combustion taught in class, and outline what does it entail for turbulent-combustion modeling.

SEE PAGE 14 OF INSTRUCTOR NOTES

+20/20

b) Draw the premixed turbulent-combustion diagram in terms of the ratio of the large turnover velocity $u'$ to the flame propagation speed $S_L^0$ versus the ratio of the integral length scale $\ell$ to flame thickness $\delta_L^0$. Identify the mean nondimensional parameters and give a brief description of each of the burning regimes in the diagram (use back of the page if needed).

SEE PAGE 16 OF INSTRUCTOR NOTES

+16 DIAGRAM

+6 PARAMETERS

+8 REGIMES

+30/30

**Student's Name:** JAVIER URZAY

**Question 2** (50 pts)

Select true (T) or false (F) for each of the statements in the list provided for each question. A complementary and *brief* mathematical proof / sketch of your answer on the back of the page would be welcome, but it is **not** needed in order to get full credit.

= MEANS CORRECT ANSWER → +50/30 EACH

**3.1** In $CH_4 - O_2$ laminar premixed flames,

a) there exists a fuel-consumption (inner) layer on the fuel side in which $H_2$ and CO are oxidized to $H_2O$ and $CO_2$ respectively (T/F)

b) there exists an oxidation layer on the oxidizer side in which $H_2$ and CO are oxidized to $H_2O$ and $CO_2$ respectively (T/F)

c) there exists a thin fuel-consumption (inner) layer in which the fuel is attacked by H atoms to form $H_2$ and CO in chain-breaking reactions; this layer has a thickness $\delta \sim 0.1\delta_L^0$, with $\delta_L^0$ the preheat thickness (T/F)

d) the typical crossover temperatures are much lower than in hydrogen combustion (T/F).

**3.2** The thermal production of $NO_x$ in premixed burners

a) is minimum for stoichiometric flames (T/F)
NEAR MAX BECAUSE TEMPERATURE IS HIGH FOR $\phi \sim 1$

b) decreases with increasing flame temperature; this is why engineers from aeronautical companies design jet-engine combustors in which the flame temperature is as high as possible (T/F)

c) is beneficial because it generates ground-level $O_3$, which protects us from the Van Allen radiation belt (T/F)

d) decreases as the mixture becomes leaner or richer (T/F) → T DECREASES

**3.3** For single-step chemistry flames in the limit of large activation energies,

a) the propagation speed of a planar laminar diffusion flame scales as $\sqrt{D/t_F}$, where $D$ is the fuel mass diffusivity and $t_F$ is the flame-transit time or characteristic residence time within the preheat region (T/F)
→ DIFFUSION FLAMES DO NOT HAVE A PROPAGATION VELOCITY

b) If both the diffusivity of the deficient reactant and the thermal diffusivity are multiplied by a factor 5 and the flame transit time is multiplied by a factor 5, then, according to large activation-energy scalings in laminar premixed flames, → $\ell_\delta$ = CONSTANT, $D_T' = 5D_T$, $t_F' = 5t_F$ → $S_L^{0\prime} \sim \left(D_T'/t_F'\right)^{1/2}$, $\delta_L^0 \sim (D_T t_F)^{1/2}$

   b1) the flame would become thinner by a factor 5 but the planar flame propagation speed would remain the same (T/F)

   b2) the flame would become thicker by a factor 5 but the planar flame propagation speed would remain the same (T/F)

   b3) the flame thickness remains the same but the planar flame propagation speed is larger by a factor $\sqrt{5}$ (T/F)

c) For flames at sufficiently small Lewis numbers, as in the case of lean hydrogen-oxygen deflagrations, the flame front remains mostly flat because of diffusive-thermal stabilizing effects (T/F)

d) the chemical reaction in premixed flames takes place in a layer which is much thinner than the preheat zone (T/F)

$\delta_f \sim \delta_L^0/\beta$ WITH $\beta \gg 1$ (ZEL'DOVICH NUMBER)

**Student's Name:** JAVIER URZAY

**3.4** In turbulent premixed flames,

a) there exists an effect called "countergradient diffusion" in which the turbulent flux of reaction-progress variable $c$ in the normal direction to the flame is directed towards regions of decreasing $c$, that is why it is called "countergradient" (T/F) INCREASING

b) direct numerical simulations and experiments show that the countergradient diffusion effect is likely to be important in regions of high turbulent intensity and, in particular, in regions in which the Kolmogorov eddies are able to penetrate in the reaction zones (T/F) LOW

c) according to the Bray-Moss-Libby model, the differences between Reynolds-averaged and Favre-averaged variables tend to increase with increasing thermal expansion (T/F)

d) Lewis number effects are irrelevant for the propagation of turbulent premixed flames because molecular diffusion is typically neglected in RANS codes (T/F) → $S_L^0$ HAS A STRONG DEPENDENCE ON $Le$

**3.5** In the modeling of turbulent premixed flames,

a) the eddy break up (EBU) model is a turbulent combustion model for the infinitely-fast chemistry limit (T/F)

b) the level set approach is used to track the propagation dynamics of turbulent diffusion flames (T/F)

c) the flame surface-density transport equation has a production term related to the generation of flame surface by curvature and a depletion term related to the destruction of flame surface by tangential strain-rate (T/F) JUST THE CONTRARY

d) the Bray-Moss-Libby model describes the crossing frequency of thick flames (T/F)

**3.6** In wrinkled premixed flames,

a) flame instabilities induced by gravity occur typically at small wavelengths (of the same order as the flame thickness) (T/F) LONG

b) there exists a diffusive thermal instability for Lewis numbers smaller than 0.5 (approximately) by which the flame front develops a cellular shape (T/F)

c) if thermal expansion is negligible, the flame is neutrally stable to Darrieus-Landau instabilities (T/F)

d) diffusive thermal instabilities can stabilize the Darrieus-Landau instability at small wavelengths (T/F)

**3.7** In the mixing of two reactants in a turbulent flow,

a) the scalar dissipation rate is always a source in the scalar variance equation (T/F) SINK

b) the scalar dissipation rate is maximum in zones where only one of the reactants exists (T/F)

e) for order-unity Schmidt numbers, the molecular mixing of two reactants typically occurs in time scales which are much longer than the integral time scale (T/F) SHORTER

f) macroscopic mixing or stirring is sufficient for having chemical reaction between reactants (T/F)

# ME 471: Turbulent Combustion, Spring 2012

**Stanford University**

**Homework 3: Non-premixed Turbulent Combustion (I)**

Due Tuesday, June 5 in class.

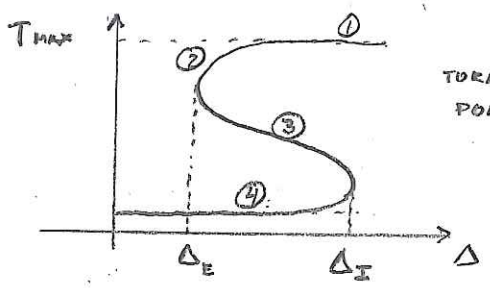
**Guidelines:** Please turn in a *neat* and *clean* homework that gives all the formulae that you have used as well as details that are required for the grader to understand your solution. Show all work. Required plots should be generated using computer software such as Matlab or similar program. Answers should be written in the blank spaces provided in these homework sheets. Use the back of the page in case you need additional space (not recommended to use more space than provided), for which a clear indication should be written to warn the reader of the presence of text there. Vector quantities are denoted in **bold** letters in what follows.

**Student's Name:** JAVIER URZAY ..... **Student's ID:** .....

**Solve Question 1 and Question 2.**

**Question 1** (50 pts)

a) Sketch the S-curve obtained by Liñán ("Asymptotic structure of counterflow diffusion flames at large activation energies", 1974) in terms of the reduced Damköhler number $\Delta$ versus the maximum temperature $T_{\max}$. Give a brief description of the physical phenomena that take place at both turning points. Locate on the graph the extinction Damköhler number $\Delta_E$ and give an explanation of its physical meaning. Finally, give a brief description of each burning regime. (25pts)




TURNING POINTS:

$\Delta_I$ : IGNITION DAMKÖHLER NUMBER +2.5

$\Delta_E$ : EXTINCTION DAMKÖHLER NUMBER (DIFFUSION TIME ~ CHEMICAL TIME) +2.5

REGIMES : SEE PAGE 9 (BACK) OF THE INSTRUCTOR NOTES FOR A DESCRIPTION OF EACH REGIME

+5 EACH

+ 25/25

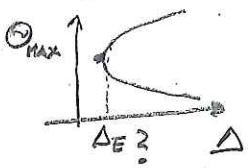
**Student's Name:** JAVIER UREÑA Y

b) In his paper, Liñán ("Asymptotic structure of counterflow diffusion flames at large activation energies", 1974) identified a critical Damköhler number for flame extinction $\Delta_E$ in the diffusion-flame regime, which is given by

$$\Delta_E = \mathrm{e}^1 \left[(1-|\gamma|) - (1-|\gamma|)^2 + 0.26(1-|\gamma|)^3 + 0.055(1-|\gamma|)^4\right]. \quad (1)$$

In particular, for $\Delta < \Delta_E$ the inner-zone equation

$$\frac{d^2\Theta}{d\eta^2} = (\Theta-\eta)(\Theta+\eta)\exp\left[-\Delta^{-1/3}(\Theta+\gamma\eta)\right] \quad (2)$$




does not have any solution. Equation (2) is subject to $d\Theta/d\eta \to \pm 1$ at $\eta \to \pm\infty$. Equation (2) describes de reactive-diffusive zone in diffusion flames at large activation energies, with $\Theta(\eta)$ being the inner temperature, $\eta$ a stretched coordinate normal to the flame, and $\Delta$ the reduced Damköhler number. Additionally, $1-\gamma$ is twice the ratio between the heat transferred from the flame towards the oxidizer side and the total chemical heat released. Therefore, $\Delta$ and $\gamma$ are external parameters in equation (2) - see class notes or Liñán (1974) paper for a formal derivation of the inner-zone equation (2) if needed -.

Provide a formal derivation of (1) by conveniently manipulating the inner-zone equation (2). (25 pts)

---

FIRST THING TO NOTICE IS THAT THE SOLUTIONS FOR $\pm\gamma$ ARE TRIVIALLY RELATED, SINCE A CHANGE OF VARIABLES IN (2) $\gamma' = -\gamma$, $\eta' = -\eta$ YIELDS EXACTLY THE SAME PROBLEM. FOR $\gamma > 0$ A PREFERENTIAL LEAKAGE OF OXIDIZER OCCURS, AND FOR $\gamma < 0$ FUEL LEAKAGE IS MORE IMPORTANT. WE WILL FOCUS ON $\gamma > 0$ AND WILL TRY TO FIND AN EXPANSION OF $\Delta_E$ IN TERMS OF THE SMALL PARAMETER $m = \frac{1-|\gamma|}{2} \ll 1$, IN SUCH A WAY THAT $\Delta_E$ ONLY DEPENDS ON $|\gamma|$ GIVEN THE SYMMETRY DESCRIBED ABOVE.

ADDITIONALLY, NOTE THAT $Y_{O_2} \sim \Delta^{-1/3}/\beta\,(\Theta - \eta)$ AND $Y_F \sim \Delta^{-1/3}/\beta\,(\Theta + \eta)$ AS OBSERVED BY USING THE INNER ASYMPTOTIC EXPANSION OF THE TEMPERATURE (EQ 70 IN LIÑÁN'S PAPER) TOGETHER WITH THE ALGEBRAIC RELATIONS (3) AND (4) FROM LIÑÁN'S PAPER.

A SMALL PARAMETER $m = \frac{1-|\gamma|}{2} \ll 1$ IS DEFINED HERE, NOTICE THAT AS $\gamma \to 1$ THE OXIDIZER LEAKAGE THROUGH THE FLAME INCREASES FOR A FIXED $\Delta$ AND BECOMES INFINITE FOR $\Delta < \Delta_E$. FOR $\gamma > 1$ THERE EXISTS A PREMIXED STRUCTURE ON THE FUEL SIDE WITH A LARGE EXCESS OF OXIDIZER, TO OBTAIN THE EXPANSION (4), ONE FIRST NEEDS TO SHIFT THE INNER COORDINATE $\eta$ TO REGIONS WHERE THE OXIDIZER MASS FRACTION BECOMES OF ORDER UNITY: $\xi = 2\eta + b/m$, WITH $b$ AN ORDER-UNITY PARAMETER (NOTICE THAT THIS REGION GOES TO INCREASINGLY POSITIVE VALUES - I.E. TO THE FUEL SIDE - AS $\gamma \to 1$). ALSO, A NEW VARIABLE $\varphi = \Theta + \eta$ IS DEFINED TO DENOTE THE INNER FUEL MASS FRACTION. IN THESE VARIABLES, EQ (2) BECOMES




$$\frac{d^2\varphi}{d\xi^2} = \frac{b}{4m}\, e^{-\Delta^{-1/3}b}\, \varphi\left[1 + (\varphi-\xi)\frac{m}{b}\right] e^{-\Delta^{-1/3}\left[\varphi - m\xi\right]}$$

SUBJECT TO $\begin{cases} \frac{d\varphi}{d\xi} \to 1 & \text{AS } \xi \to +\infty \\ \frac{d\varphi}{d\xi} \to 0 & \text{AS } \xi \to -\infty. \end{cases}$

IT IS MORE EXPEDIENT TO RESCALE $\varphi$ AND $\xi$ AS $\tilde{\varphi} = \varphi\Delta^{-1/3}$ AND $\tilde{\xi} = \xi\Delta^{-1/3}$, WITH $\tilde{b} = b\Delta^{-1/3}$, IN SUCH A WAY THAT THE DAMKÖLER NUMBER IS DROPPED FROM THE EXPONENTIAL:

$$\frac{d^2\varphi}{d\xi^2} = \delta\,\varphi\left[1+(\varphi-\xi)\frac{m}{b}\right]e^{-(\varphi-m\xi)}, \quad \text{SUBJECT TO} \quad \begin{cases} \frac{d\varphi}{d\xi}\to 1 \text{ AS } \xi\to+\infty \\ \frac{d\varphi}{d\xi}\to 0 \text{ AS } \xi\to-\infty \end{cases}$$

WHERE THE TILDES HAVE BEEN DROPPED. EXPANDING $\varphi$ AND $\delta = \frac{b\Delta}{4m}e^{-b}$ IN POWERS OF $m$:

$$\left.\begin{aligned}\varphi &= \varphi_0 + m\varphi_1 + O(m^2)\\ \delta &= \delta_0 + m\delta_1 + O(m^2)\end{aligned}\right\}$$ ONE OBTAINS, TO LEADING ORDER:

$$\frac{d^2\varphi_0}{d\xi^2} = \delta_0\varphi_0 e^{-\varphi_0} \quad \text{SUBJECT TO} \quad \frac{d\varphi_0}{d\xi}\to 1 \text{ AS } \xi\to+\infty \ (\varphi_0\sim\xi+\cancel{c}^{\,0}\to\text{FROM OUTER SOL.}), \text{ AND } \frac{d\varphi_0}{d\xi}\to 0 \text{ AS } \xi\to-\infty \ (\varphi\to\cancel{c}^{\,0}\to\text{FROM OUTER SOL.})$$

SINCE $\frac{d^2\varphi_0}{d\xi^2} = \frac{1}{2}\frac{d}{d\varphi_0}\left(\frac{d\varphi_0}{d\xi}\right)^2 = \delta_0\varphi_0 e^{-\varphi_0}$, INTEGRATING THIS EQUATION BETWEEN $\varphi_0=0$ AND $\varphi_0\to+\infty$, ONE OBTAINS THAT $\underline{\underline{\delta_0 = 1/2}}$, WHERE USE OF THE RESULT $\int_0^{+\infty}\varphi_0 e^{-\varphi_0}d\varphi_0 = 1$ HAS BEEN MADE. SIMILARLY, IN THE SECOND APPROXIMATION, THE PROBLEM

$$\frac{d^2\varphi_1}{d\xi^2} - \delta_0\varphi_1(1-\varphi_0)e^{-\varphi_0} = \delta_0\varphi_0 e^{-\varphi_0}\left[\xi + k + \frac{\varphi_0-\xi}{b}\right] \quad (*)$$

SUBJECT TO $\frac{d\varphi_2}{d\xi}\to 0$ AT $\xi\to\pm\infty$ IS FOUND, WITH $k = \delta_1/\delta_0$. THE HOMOGENEOUS SOLUTION OF THIS EQUATION IS SIMPLY $\varphi_{1h} = \frac{d\varphi_0}{d\xi}$ SINCE $\frac{d\varphi_1}{d\xi} = \frac{d^2\varphi_0}{d\xi^2} = \varphi_0\delta_0 e^{-\varphi_0}$ AND $\frac{d^2\varphi_1}{d\xi^2} = \delta_0\varphi_0' e^{-\varphi_0} - \varphi_0\delta_0\varphi_0' e^{-\varphi_0} = \delta_0\varphi_1 e^{-\varphi_0}(1-\varphi_0)$. MULTIPLYING $(*)$ BY $\varphi_{1h}$ AND USING THAT $\varphi_{1h}'' - \delta_0\varphi_{1h}(1-\varphi_0)e^{-\varphi_0} =$ ONE OBTAINS

$$\underbrace{\varphi_{1h}\varphi_1'' - \varphi_{1h}''\varphi_1}_{(\varphi_{1h}\varphi_1' - \varphi_{1h}'\varphi_1)'} + \cancel{\varphi_1''\varphi_{1h}} - \cancel{\delta_0\varphi_1(1-\varphi_0)}e^{-\varphi_0}\varphi_{1h} = \delta_0\varphi_0\varphi_{1h}e^{-\varphi_0}\left[\xi + k + \frac{\varphi_0-\xi}{b}\right],$$

THEREFORE:

$$\frac{d}{d\xi}\left(\frac{d\varphi_1}{d\xi}\frac{d\varphi_0}{d\xi} - \frac{d^2\varphi_0}{d\xi^2}\varphi_1\right) = \delta_0\varphi_0\frac{d\varphi_0}{d\xi}e^{-\varphi_0}\left[\xi + k + \frac{\varphi_0-\xi}{b}\right],$$

INTEGRATING FROM $\xi=-\infty$ TO $+\infty$, AND APPLYING BOUNDARY CONDITIONS ONE OBTAINS

$$\int_{-\infty}^{+\infty}\delta_0\varphi_0\frac{d\varphi_0}{d\xi}e^{-\varphi_0}\left[\xi + k + \frac{\varphi_0-\xi}{b}\right]d\xi = 0 \quad \text{AS A SOLVABILITY CONDITION},$$

WHICH CAN BE SPLIT INTO THE FOLLOWING INTEGRALS:

$$\int_0^{+\infty}\varphi_0 k e^{-\varphi_0}d\varphi_0 + \int_0^{+\infty}\frac{\varphi_0^2}{b}e^{-\varphi_0}d\varphi_0 + \left(1-\frac{1}{b}\right)\int_{-\infty}^{+\infty}\varphi_0 e^{-\varphi_0}\frac{d\varphi_0}{d\xi}\xi d\xi = 1$$

(1) (2) (3)

WITH (1) $= k$, (2) $= 2/b$, (3) $= \zeta\left(1-1/b\right)$ WITH $\zeta = \int_{-\infty}^{+\infty}\varphi_0 e^{-\varphi_0}\frac{d\varphi_0}{d\xi}\xi\,d\xi$ A CONSTANT THAT NEEDS TO BE OBTAINED NUMERICALLY. THE SOLVABILITY CONDITION FOR THE SECOND ORDER THEN REDUCES TO:

$$k + \zeta + (2-\zeta)/b = 0 \Rightarrow k = (\zeta-2)/b - \zeta = \delta_1/\delta_0 \Rightarrow \delta_1 = \frac{(\zeta-2)}{2b} - \zeta/2.$$

THE TWO-TERM EXPANSION OF $\delta$ BECOMES: $\delta = \frac{b\Delta}{4m}e^{-b} = \frac{1}{2}\left[1 - \left(\zeta - \left(\frac{\zeta-2}{b}\right)\right)m + O(m^2)\right]$

BY PERFORMING $\frac{d\Delta}{db} = 0$, A VALUE $b = 1 + O(m)$ IS OBTAINED, WHICH MAKES $\Delta$ TO BE MINIMUM: $\Delta = \Delta_E$. IN THIS WAY, THE TWO-TERM EXPANSION OF $\Delta_E$ CAN BE WRITTEN AS

$$\Delta_E = 2em(1-2m) = e\left\{(1-|\delta|) - (1-|\delta|)^2\right\}.$$ FROM A NUMERICAL INTEGRATION OF (2) (SEE FIG 8 OF LIÑÁN'S PAPER), ONE CAN OBTAIN THAT $\Delta_E = 0.856$ FOR $\gamma=0$. USING THIS CONDITION AND THE SYMMETRY OF $\Delta_E$ AT $\gamma=0$ ($d\Delta_E/d\gamma = 0$ AT $\gamma=0$, SEE FIG 12 OF LIÑÁN'S PAPER), THE THIRD AND FOURTH ORDERS OF THE EXPANSION OF $\Delta_E$ CAN BE OBTAINED, WHICH YIELDS $\Delta_E = e\left\{(1-|\delta|) - (1-|\gamma|)^2 + 0.26(1-|\gamma|)^3 + 0.055(1-|\gamma|)^4\right\}$

Student's Name: JAVIER URZAY

**Question 2** (50 pts)

For a steady laminar counterflow diffusion flame with constant density and equal diffusivities of fuel and oxidizer,

a) Prove that the scalar dissipation rate $\chi = D|\nabla Z|^2$ can be written as

$$\chi = \frac{a}{2\pi} \exp\left[-2(\mathrm{erfc}^{-1}(2Z))^2\right] \tag{3}$$

where $Z$ is the mixture fraction, $a$ is the strain rate, and $\mathrm{erfc}(p) = (2/\sqrt{\pi}) \int_p^\infty \mathrm{e}^{-t} dt$ is the complementary error function.

SOL: LOOK AT PAGE 9 OF THE INSTRUCTOR NOTES FOR DERIVATION OF (3).

+30

b) What is the physical meaning of the scalar dissipation rate at stoichiometry $\chi_{st} = \chi(Z = Z_{st})$? In this formulation, $Z_{st}$ is the stoichiometric mixture fraction.

IT REPRESENTS THE INVERSE OF THE DIFFUSION TIME THROUGH THE STOICHIOMETRIC SURFACE.

+5

c) Using (3), prove that $\chi_{st}$ is of order $aZ_{st}^2$ when $Z_{st} \ll 1$. This result is valid for hydrocarbon-air flames, in which $Z_{st}$ is typically a small number. According to this result, is the diffusion time through the stoichiometric surface much larger or much smaller than the characteristic strain time?

SINCE $Z = \frac{1}{2}\mathrm{erfc}\left(\frac{z}{\sqrt{2}}\right) \sim \frac{1}{\sqrt{2\pi}} \frac{e^{-z^2/2}}{z}$ FOR LARGE $z$, AND $\chi = a\left(\frac{dz}{d\hat{z}}\right)^2 \sim \frac{a}{2\pi}\left(-e^{-\frac{z^2}{2}}\right)^2$ (DIMENSIONLESS!)

THEN $\chi \sim a Z^2 z^2 = 2a Z^2 \underbrace{\mathrm{erfc}^{-1}(2Z^2)}_{O(1) \text{ WHEN } Z \to Z_{st}} \Rightarrow \chi_{st} \sim 2a Z_{st}^2$

+10

ALSO, SINCE $\chi_{st} \sim \frac{1}{t_{d_{st}}} \sim a Z_{st}^2$, THEN $t_{d_{st}} \gg \frac{1}{a}$ $\Rightarrow$ THE DIFFUSION TIME THROUGH THE STOICHIOMETRIC SURFACE IS MUCH LARGER THAN THE STRAIN TIME FOR $Z_{st} \ll 1$ SINCE $Z = Z_{st}$ IS LOCATED DEEP INSIDE THE AIR SIDE.

+5

# ME 471: Turbulent Combustion, Spring 2012

**Stanford University**

**Final Exam**

Tuesday, June 12

**Part I: Questions**
**(closed books, closed notes, no calculator allowed)**
**30 minutes**

**Guidelines:** Please turn in a *neat* and *clean* exam solution. Answers should be written in the blank spaces provided in these exam sheets. Vector quantities are denoted in **bold** letters in what follows.

**Student's Name:** JAVIER URIAY ..... **Student's ID:** .....

**Question 1** (25 pts)

Explain the concept of steady flamelet models in non-premixed turbulent combustion, and how are they typically implemented in RANS of turbulent diffusion flames.

SEE PAGE 26 AND FIGS 5 + 6 OF THE INSTRUCTOR NOTES

+25

**Student's Name:** JAVIER URZAY

**Question 2** (25 pts)

Select true (T) or false (F) for each of the statements in the list provided for each question, or fill in the gaps when indicated by the symbol (.....). A complementary and *brief* mathematical proof / sketch of your answer on the back of the page would be welcome, but it is **not** needed in order to get full credit.

**2.1** In the mixing of two reactants in a turbulent flow,

a) the scalar dissipation rate is always a sink in the equation for the mean (T/F)

b) the scalar dissipation rate is minimum in zones where only one of the reactants exists (T/F)

e) for order-unity Schmidt numbers, the molecular mixing of two reactants typically occurs in time scales which are much shorter than the integral time scale (T/F)

f) For chemical reactions to occur in combustion, fuel and oxidizer must be mixed at the (MOLECULAR) level.

**2.2** For single-step chemistry flames in the limit of large activation energies,

a) the strain rate at extinction of a laminar diffusion flame scales as $\sqrt{D/t_F}$, where $D$ is the fuel mass diffusivity and $t_F$ is the flame-transit time or characteristic residence time within the preheat region (T/F)

b) at diffusion-flame extinction in counterflow mixing layers, the diffusion time through the mixing layer is of the same order as the flame transit time through the preheat region of a stoichiometric laminar planar premixed flame (T/F)

c) the scalar dissipation rate at stoichiometry $\chi_{st}$ represents the (INVERSE OF THE DIFFUSION TIME) through the stoichiometric surface.

d) the characteristic reaction-zone thickness in diffusion flames is of order ($\Delta^{-1/3}\delta_M$), where ($\Delta$) is the (DAMKÖHLER) number, ($\delta$) is the (ZEL'DOVICH) number, and ($\delta_M$) is the (MIXING LAYER) thickness.

**2.3** In turbulent non-premixed flames,

a) the mixture fraction is a conserved scalar because (IT IS NEITHER DESTROYED OR GENERATED BY CHEMICAL REACTIONS).

b) the flamelet-progress-variable-approach (FPVA), a mostly unique mapping of all tabulated chemical states is provided in terms of mixture fraction and progress variable (T/F)

c) the Burke-Schumann approximation is accurate for calculating extinction of turbulent diffusion flames (T/F)

d) the problem $\rho\chi(Z)d^2\phi/dZ^2 = \dot{w}_\phi$, for any scalar $\phi$, and with $\chi$ the scalar dissipation rate and $Z$ the mixture fraction, represents a convection-diffusion problem (T/F)

e) the probability density function for the mixture fraction is typically modeled by using a (BETA) function.

+ 25/19 EACH

# ME 471: Turbulent Combustion, Spring 2012

**Stanford University**

**Final Exam**

Tuesday, June 12

**Part II: Problem**
**(open books, open notes, calculator allowed)**
**1 hour 30 minutes**

**Guidelines:** Please turn in a *neat* and *clean* exam solution. Answers should be written in the blank spaces provided in these exam sheets. Vector quantities are denoted in **bold** letters in what follows.

**Student's Name:** JAVIER URZAY ..... **Student's ID:** .....

**Problem** (50 pts)

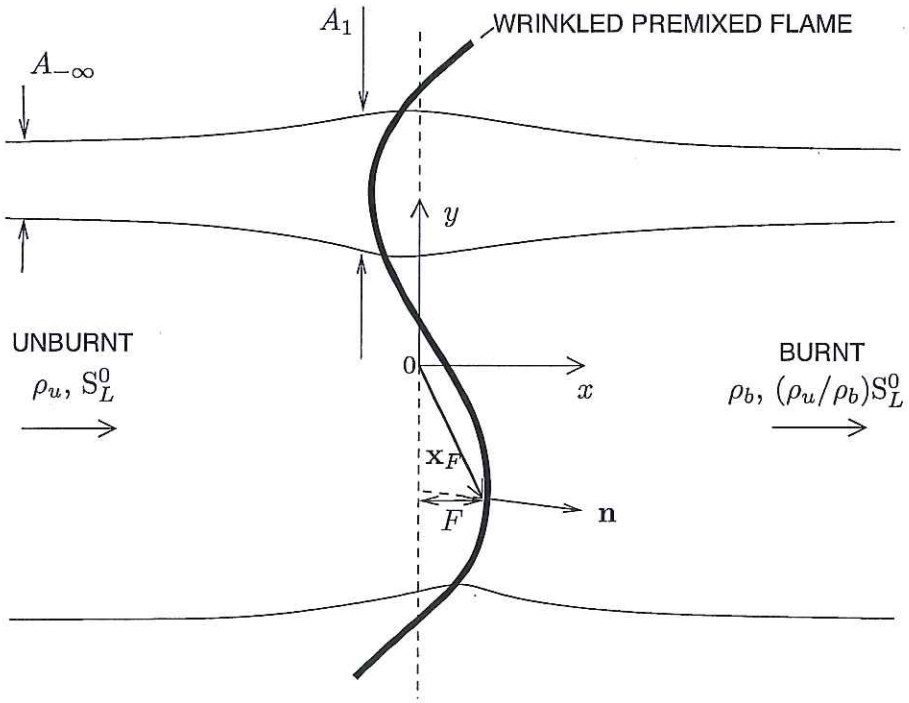



Figure 1: Schematics of the problem

In the hydrodynamic or "Darrieus-Landau" instability of premixed flames, a stream tube with cross-sectional area $A_{-\infty}$ and upstream flow velocity $u_{-\infty} = S_L^0$ widens due to flow divergence ahead of the flame, with $S_L^0$ the planar propagation velocity. This divergence effect is generated by the thermal expansion at the front that induces a flow component normal to the flame contour. The streamlines become deflected as they cross the front. At large distances from the front, the streamlines are parallel again, but the downstream velocity is $u_\infty = (\rho_u/\rho_b)u_{-\infty} > u_{-\infty}$. At the cross section $A_1$, where the density is still equal to unburnt density $\rho_u$, the flow velocity is $u_1 = (A_{-\infty}/A_1)u_{-\infty} < u_{-\infty}$ because of mass conservation. Since the unperturbed flame propagates with $u_{-\infty}$, the burning velocity is larger than $u_1$ and the flame will propagate upstream, thereby enhancing the initial perturbation.

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In the thin-flame limit, in which the flame is treated as a gasdynamic discontinuity, the parameter $\epsilon = k\delta_L^0 \ll 1$ is small, in that the characteristic wavelength of the transverse flame corrugations, $\lambda = 2\pi/k$, with $k$ the wavenumber, is much larger than the unperturbed flame thickness $\delta_L^0$. In the limit $\epsilon \to 0$, the infinitesimally thin flame separates the burnt and unburnt regions, in which the density is constant ($\rho = \rho_u$ in the unburnt zone and $\rho = \rho_b$ in the burnt zone) and in which molecular transport is negligible.

In this problem, the Darrieus-Landau instability is studied in the presence of curvature-correction effects (a.k.a. diffusive-thermal effects) on the propagation velocity, which here is assumed to be given by the linear relationship $S_L = S_L^0(1-\mathcal{L}\kappa)$, where $S_L^0$ is the planar propagation velocity on the unburnt side, $\mathcal{L}$ is a Markstein length and $\kappa$ is the local curvature. In order to obtain a dispersion equation that relates the growth rate $\sigma$ of the instability with the wavenumber $k$, the thermal-expansion ratio $\alpha = (\rho_u - \rho_b)/\rho_u$ and the Markstein length $\mathcal{L}$, follow the next steps:

1.1 Write down the continuity and momentum conservation equations for the $x-$ and $y-$ components of the flow velocity $\mathbf{v} = u\mathbf{e_x} + v\mathbf{e_y}$, with $\mathbf{e_i}$ unit vectors. Use dimensionless variables $\mathbf{v}^\star = \mathbf{v}/S_L^0$, $\rho^\star = \rho/\rho_u$, $P^\star = P/\rho_u(S_L^0)^2$, $\mathbf{x}^\star = \mathbf{x}/\delta_L^0$ and $t^\star = t/t_F$. In this formulation, $\delta_L^0 = S_L^0 t_F$ is the flame thickness, $t_F$ is the flame-transit time, $P$ is the pressure and the remaining symbols are defined in the problem statement.

MOLECULAR TRANSPORT IS NEGLIGIBLE
ON THE BURNT AND UNBURNT ZONES
$+\ \rho = \rho_u$ ON THE UNBURNT REGION
$+\ \rho = \rho_b$ ON THE BURNT REGION

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = -\frac{\partial P}{\partial x}$$

$$\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) = -\frac{\partial P}{\partial y}$$

+2.5

1.2 What are the boundary conditions for the velocity at $x \to \pm\infty$?

AT $\underline{x} \to +\infty$, $\underline{v} = \frac{\rho_u S_L^0}{\rho_b}\underline{e_x}$ ; AT $\underline{x} \to -\infty$, $\underline{v} = S_L^0\underline{e_x}$ +2.5

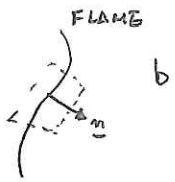
1.3 In the limit $\epsilon \to 0$, the equations written in part 1.1. are only valid on both sides of the flame because of thermal expansion, which induces an infinite density gradient in the first approximation. Jump conditions for the velocity and pressure can be derived in the following manner:

1.3.1 If $\mathbf{x}_F$ is the flame position and $\mathbf{n}$ is the unit normal vector to the front towards the burnt side (see Fig.1), write an equation that states the continuity of the burning rate $\dot{m} = \rho S_L$ across the flame in terms of the relative velocity $(\mathbf{v} - d\mathbf{x}_F/dt)\cdot\mathbf{n}$ on both sides of the flame. (Note: Recall that if $d\mathbf{x}_F/dt$ is the flame speed in the laboratory frame, then the kinematic balance requires that $S_L = (\mathbf{v} - d\mathbf{x}_F/dt)\cdot\mathbf{n}$ on the unburnt region.)

$$\rho_u\left(\underline{v}^{(u)} - \frac{d\underline{x}_F}{dt}\right)\cdot\underline{n} = \rho_b\left(\underline{v}^{(b)} - \frac{d\underline{x}_F}{dt}\right)\cdot\underline{n}$$

+2.5

1.3.2 Additionally, write a momentum balance equation across the flame in terms of the relative velocity $(\mathbf{v} - d\mathbf{x}_F/dt)\cdot\mathbf{n}$ and pressure on both sides of the flame.




$$-\rho_u \underline{v}^{(u)}\left[\underline{v}^{(u)} - \frac{d\underline{x}_F}{dt}\right]\cdot\underline{n} + \rho_b \underline{v}^{(b)}\left[\underline{v}^{(b)} - \frac{d\underline{x}_F}{dt}\right]\cdot\underline{n} = \left(P^{(u)} - P^{(b)}\right)\cdot\underline{n}$$

+2.5

**Student's Name:** JAVIER URZAY

1.3.3 Use the the thermal-expansion coefficient $\alpha = (\rho_u - \rho_b)/\rho_u$ and the nondimensional variables defined above in order to express the equations obtained in 1.3.1 and 1.3.2 in dimensionless form.

SINCE $\frac{\rho_b}{\rho_u} = -\frac{\rho_u + \rho_u + \rho_b}{\rho_u} = 1 - \alpha$, THE JUMP CONDITIONS BECOME

$$-\alpha \frac{dx_F}{dt} = (1-\alpha)\,\underline{v}^{(b)}\cdot\underline{n} - \underline{v}^{(u)}\cdot\underline{n}$$

+2.5

$$\frac{dx_F}{dt}\cdot\underline{n}\left(\underline{v}^{(u)} - (1-\alpha)\underline{v}^{(b)}\right) = \underline{v}^{(u)}\underline{v}^{(u)}\cdot\underline{n} - (1-\alpha)\underline{v}^{(b)}\underline{v}^{(b)}\cdot\underline{n} + \left(P^{(u)} - P^{(b)}\right)\underline{n}$$

1.3.4 By employing the ansatz $G = x - F(y,t) = G_0$ at the flame, with $G_0$ a constant and $F(y,t)$ the displacement function, show that the scalar product $\mathbf{n}\cdot d\mathbf{x}_F/dt$ can be written as

$$\mathbf{n}\cdot\frac{d\mathbf{x}_F}{dt} = \frac{F_t}{\sqrt{1+F_y^2}}, \tag{1}$$

where $F_t = \partial F/\partial t$ and $F_y = \partial F/\partial y$.

SINCE $\dot{\underline{x}}_F = \dot{x}_F\underline{e}_x + \dot{y}_F\underline{e}_y$, WITH $0 = \dot{x}_F - F_t - F_y\dot{y}_F$ FROM THE ANSATZ, AND ALSO

$\underline{n} = \frac{\nabla G}{|\nabla G|} = \frac{\underline{e}_x - F_y\underline{e}_y}{(1+F_y^2)^{1/2}}$, THEN $\dot{\underline{x}}_F\cdot\underline{n} = \frac{\dot{x}_F - F_y\dot{y}_F}{(1+F_y^2)^{1/2}} = \frac{F_t}{(1+F_y^2)^{1/2}}$

+2.5

1.3.5 Use equation (1) derived above to show that the jump conditions obtained in part 1.3.3 can be expressed as

$$\alpha F_t = u^{(u)} - (1-\alpha)u^{(b)} - F_y\left[v^{(u)} - (1-\alpha)v^{(b)}\right], \tag{2}$$

$$F_t\left[u^{(u)} - (1-\alpha)u^{(b)}\right] = u^{(u)}\left(u^{(u)} - F_y v^{(u)}\right) - (1-\alpha)u^{(b)}\left[u^{(b)} - F_y v^{(b)}\right] + P^{(u)} - P^{(b)}, \tag{3}$$

$$F_t\left[v^{(u)} - (1-\alpha)v^{(b)}\right] = v^{(u)}\left(u^{(u)} - F_y v^{(u)}\right) - (1-\alpha)v^{(b)}\left[u^{(b)} - F_y v^{(b)}\right] - (P^{(u)} - P^{(b)})F_y, \tag{4}$$

where the superindexes $^{(u)}$ and $^{(b)}$ denote variables evaluated on the unburnt and burnt sides, respectively.

DIRECT PROOF BY SUBSTITUTING (1) IN THE JUMP CONDITIONS AND DECOMPOSING THE MOMENTUM BALANCE INTO X AND Y COMPONENTS.

+2.5

1.4 For $\epsilon \ll 1$, the velocity components, the pressure and the displacement function may be expanded in power series of $\epsilon$ as

$$u = U_0 + \epsilon U_1 + O(\epsilon^2), \quad v = \epsilon V_1 + O(\epsilon^2), \quad P = P_0 + \epsilon P_1 + O(\epsilon^2), \quad \text{and} \quad F = \epsilon F_1 + O(\epsilon^2). \tag{5}$$

Similarly, a coordinate transformation

$$x = \xi + F(\eta,\tau), \quad y = \eta, \quad \text{and} \quad t = \tau \tag{6}$$

becomes useful in order to set the flame and the jump conditions at $\xi = 0$.

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Use these expansions prove that, to leading order, the jump conditions derived in part 1.3.5 reduce to

$$U_0^{(u)} = 1, \quad U_0^{(b)} = 1/(1-\alpha), \quad \text{and} \quad P_0^{(u)} - P_0^{(b)} = \alpha/(1-\alpha). \tag{7}$$

TO LEADING ORDER, THE JUMP CONDITIONS IN (2)-(4) BECOME

$$U_0^{(u)} - U_0^{(b)}(1-\alpha) = 0 \Rightarrow U_0^{(u)} = 1, \quad U_0^{(b)} = \frac{1}{1-\alpha}$$ 2.5

AND $$0 = U_0^{(u)2} - (1-\alpha) U_0^{(b)2} + P_0^{(u)} - P_0^{(b)} \Rightarrow P_0^{(u)} - P_0^{(b)} = \frac{\alpha}{1-\alpha}$$ 2.5

1.5 Use the asymptotic expansions (5) and the coordinate transformation (6) to show that the jump conditions (2)-(4) reduce to

$$\alpha F_{1\tau} = U_1^{(u)} - (1-\alpha)U_1^{(b)}, \tag{8}$$

$$P_1^{(u)} - P_1^{(b)} = 2(U_1^{(b)} - U_1^{(u)}), \tag{9}$$

$$V_1^{(u)} - V_1^{(b)} = \frac{\alpha F_{1\eta}}{1-\alpha}, \tag{10}$$

+2.5

IN THE SECOND APPROXIMATION

(2) BECOMES $\alpha F_{1\xi} = V_1^{(u)} - (1-\alpha) V_1^{(b)}$

(3) BECOMES $0 = 2U_0^{(u)}U_1^{(u)} - 2(1-\alpha) U_0^{(b)} U_1^{(b)} + P_1^{(u)} - P_1^{(b)} \rightarrow P_1^{(u)} - P_1^{(b)} = 2\left(U_1^{(b)} - U_1^{(u)}\right)$

(4) BECOMES : $0 = V_1^{(u)} U_0^{(u)} - (1-\alpha) V_1^{(b)} U_0^{(b)} - \left(P_0^{(u)} - P_0^{(b)}\right) F_{1\eta}$

$$\Rightarrow V_1^{(u)} - V_1^{(b)} = \frac{\alpha}{1-\alpha} F_{1\eta}$$

1.6 Use the asymptotic expansions (5) and the coordinate transformation (6) to obtain the second approximation of the asymptotic expansion of the conservation equations written in part 1.1.

$$\left.\begin{aligned} &\frac{\partial U_1}{\partial \xi} + \frac{\partial V_1}{\partial \eta} = 0 \\ &\beta\left(\frac{\partial U_1}{\partial \tau} + U_0 \frac{\partial U_1}{\partial \xi}\right) = -\frac{\partial P_1}{\partial \xi} \\ &\beta\left(\frac{\partial V_1}{\partial \tau} + U_0 \frac{\partial V_1}{\partial \xi}\right) = -\frac{\partial P_1}{\partial \eta} \end{aligned}\right\}$$ 2.5

1.7 If all perturbations vanish far away from the flame, what are the boundary conditions for $U_1$, $V_1$ and $P_1$ at $\xi \to \pm\infty$?

$U_1, V_1, P_1 \to 0$ AT $\xi \to \pm\infty$ 2.5

1.8 To analyze the stability of the solution of the problem obtained in part 1.6, assume a normal mode decomposition for the velocity and pressure disturbances:

$$\begin{pmatrix} U_1 \\ V_1 \\ P_1 \end{pmatrix} = \begin{pmatrix} \hat{U}_1 \\ \hat{V}_1 \\ \hat{P}_1 \end{pmatrix} \exp(\gamma\xi) \exp(\sigma\tau - ik\eta) \tag{11}$$

where $\hat{U}_1$, $\hat{V}_1$ and $\hat{P}_1$ are constants, $\sigma$ is a growth rate and $k$ is the wavenumber of the transverse perturbations. The parameter $\gamma$ is obtained from imposing the boundary conditions stated in part 1.7.

**Student's Name:** JAVIER URZAY

To obtain $\gamma$, substitute (11) into the conservation equations written in part 1.6. You may have to solve the determinant of the coefficient matrix and use the boundary conditions stated in part 1.7 and the leading-order jump conditions for $U_0$ obtained in part 1.4.

$U_1 = \hat{U}_1 e^{\gamma\xi} e^{\sigma\tau - ik\eta}$, $V_1 = \hat{V}_1 e^{\gamma\xi} e^{\sigma\tau - ik\eta}$, $P_1 = \hat{P}_1 e^{\gamma\xi} e^{\sigma\tau - ik\eta}$ ⟹ SUBSTITUTING IN 1.6:

$$\begin{pmatrix} \gamma & -ik & 0 \\ \sigma + U_0\gamma & 0 & \gamma/\xi \\ 0 & \sigma + U_0\gamma & -ik/\xi \end{pmatrix} \begin{pmatrix} \hat{U}_1 \\ \hat{V}_1 \\ \hat{P}_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \iff \det(A) = 0$$

$\Rightarrow \frac{1}{\xi}(k^2 - \gamma^2)(\sigma + U_0\gamma) = 0$, WITH $U_0^{(u)} = 1$ AND $U_0^{(b)} = 1/(1-\kappa)$

+2.5

THEN $\gamma_1 = k$ $(\xi < 0)$, $\gamma_2 = -\sigma(1-\kappa)$ $(\xi > 0)$, $\gamma_3 = -k$ $(\xi > 0)$ ARE THE ONLY VALUES THAT SATISFY THE BCS.

1.9 Using the three values of $\gamma_i$ $(i = 1, 2, 3)$ obtained in part 1.8, calculate the corresponding eigenvectors $\mathbf{w}_i = (\hat{U}_{1,i}, \hat{V}_{1,i}, \hat{P}_{1,i})$ and the perturbations $U_1$, $V_1$ and $P_1$ on both sides of the flame.

EIGENVECTORS: $\gamma_1 = k$ $(\xi < 0)$

$$\begin{pmatrix} k & -ik & 0 \\ \sigma + k & 0 & k \\ 0 & \sigma + k & -ik \end{pmatrix} \begin{pmatrix} w_{11} \\ w_{12} \\ w_{13} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$\Rightarrow \underline{w}_1 = a \begin{pmatrix} 1 \\ -i \\ -1 - \sigma/k \end{pmatrix}$ +2.5

$\gamma_2 = -k$ $(\xi > 0)$

$$\begin{pmatrix} -k & -ik & 0 \\ \sigma - k & 0 & -k \\ 1-k & & 1-\kappa \\ 0 & \sigma - k & -ik \\ & 1-\kappa & 1-\kappa \end{pmatrix} \begin{pmatrix} w_{12} \\ w_{22} \\ w_{32} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$\underline{w}_2 = b \begin{pmatrix} 1 \\ +i \\ -1 + \frac{(1-\kappa)\sigma}{k} \end{pmatrix}$

$\gamma_3 = -\sigma(1-\kappa)$ $(\xi > 0)$

$$\begin{pmatrix} -\sigma(1-\kappa) & -ik & 0 \\ 0 & 0 & -\sigma \\ 0 & 0 & -\frac{ik}{(1-\kappa)} \end{pmatrix} \begin{pmatrix} w_{13} \\ w_{23} \\ w_{33} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$\underline{w}_3 = c \begin{pmatrix} 1 \\ i(1-\kappa)\sigma/k \\ 0 \end{pmatrix}$

THEN: $U_1 = a e^{k\xi} e^{\sigma\tau - ik\eta}$, $V_1 = -ia\, e^{k\xi} e^{\sigma\tau - ik\eta}$, $P_1 = -(1 + \sigma/k) a e^{k\xi} e^{\sigma\tau - ik\eta}$ FOR $\xi < 0$

$U_1 = [b e^{-k\xi} + c e^{-\sigma(1-\kappa)\xi}] e^{\sigma\tau - ik\eta}$, $V_1 = [+ib e^{-k\xi} + i(1-\kappa)\sigma/k\, c e^{-\sigma(1-\kappa)\xi}] e^{\sigma\tau - ik\eta}$, $P_1 = [-(1 - (1-\kappa)\frac{\sigma}{k}) b e^{-\sigma(1-\kappa)\xi}] e^{\sigma\tau - ik\eta}$ FOR $\xi$

1.10 Since, as stated above, in this analysis the propagation velocity $S_L$ is a function of the curvature $\kappa$, $S_L = S_L^0(1 - \mathcal{L}\kappa)$, or equivalently,

$$\left(\mathbf{v}^{(u)} - \frac{d\mathbf{x}_F}{dt}\right) \cdot \mathbf{n} = (1 - \alpha)\left(\mathbf{v}^{(b)} - \frac{d\mathbf{x}_F}{dt}\right) \cdot \mathbf{n} = 1 - \mathrm{Ma}\kappa \tag{12}$$

in dimensionless notation, answer the following questions:

1.10.1 What is the definition and physical meaning of the Markstein number Ma in this formulation?

SINCE DISTANCES ARE NONDIMENSIONALIZED WITH $\delta_L^0$, THEN $\delta_L^0 k = k^*$ IS THE DIMENSIONLESS CURVATURE AND $\mathrm{Ma} = \frac{\mathcal{L}}{\delta_L^0}$ IS THE RATIO OF THE MARKSTEIN LENGTH TO THE FLAME THICKNESS +2.5

1.10.2 Prove that the flame curvature $\kappa = -\nabla \cdot \mathbf{n}$ can be written as

$$\kappa = \frac{F_{\eta\eta}}{(1 + F_\eta^2)^{3/2}}. \tag{13}$$

SINCE $\underline{n} = \frac{e_x - F_y e_y}{(1 + F_y^2)^{1/2}}$ THEN $\kappa = -\nabla \cdot \underline{n} = \frac{F_{yy}(1 + F_y^2) - F_y^2 F_{yy}}{(1 + F_y^2)^{3/2}} = \frac{F_{yy}}{(1 + F_y^2)^{3/2}} = \frac{F_{\eta\eta}}{(1 + F_\eta^2)^{3/2}}$ +2.5

1.10.3 Using the expansions (5), and the results (12) and (13), prove that the velocity perturbations are related to $F$ by the equations

$$U_1^{(u)} = F_{1\tau} - \mathrm{Ma} F_{1\eta\eta}, \quad \text{and} \quad U_1^b = F_{1\tau} - \frac{\mathrm{Ma} F_{1\eta\eta}}{1 - \alpha} \tag{14}$$

on both sides of the flame.

TO LEADING ORDER (12) BECOMES $U_0^{(u)} = (1 - \kappa) U_0^{(b)} = 1$

AND TO SECOND ORDER: $U_1^{(u)} - F_{1t} = (1 - \kappa)(U_1^{(b)} - F_{1t}) = -\mathrm{Ma} F_{1\eta\eta}$

$\Rightarrow \begin{cases} U_1^{(u)} = F_{1t} - \mathrm{Ma} F_{1\eta\eta} \\ U_1^{(b)} = F_{1t} - \frac{\mathrm{Ma} F_{1\eta\eta}}{1 - \alpha} \end{cases}$ +2.5

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DOG | DEFINING $F_1 = \hat{F}_1 e^{\sigma t - i k x}$

1.11 Finally, obtain the dispersion relation $\sigma = \sigma(k, \alpha, \mathrm{Ma})$ by i) substituting the perturbations obtained in part 1.9 into the jump conditions (8)-(10), ii) using relations (14), and iii) solving the resulting linear system.

FOLLOWING THE PROCEDURE ABOVE, THE SYSTEM OF EQUATIONS

$$\left.\begin{aligned} a &= \sigma \hat{F}_1 + k^2 \mathrm{Ma}\, \hat{F}_1 \\ b + c &= \sigma \hat{F}_1 + k^2 \mathrm{Ma}\, \hat{F}_1 / 1-\alpha \\ a + b + (1-\alpha)\frac{\sigma}{k} c &= \frac{\alpha k \hat{F}_1}{1-\alpha} \\ 0 &= 2c + a\left(\frac{\sigma}{k} - 1\right) + b\left(1 + (1-\alpha)\frac{\sigma}{k}\right) \end{aligned}\right\}$$

WHICH CAN BE SOLVED FOR

$$\hat{a} = \frac{a}{\hat{F}_1}, \quad \hat{b} = \frac{b}{\hat{F}_1}, \quad \hat{c} = \frac{c}{\hat{F}_1} \quad \text{AND} \quad \sigma = \sigma(k)$$

TO GIVE

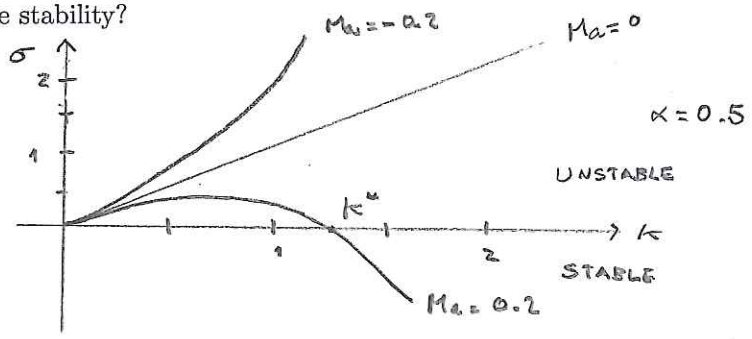
$$\sigma = \frac{k}{2-\alpha}\left\{\left(1 + k^2\mathrm{Ma}^2 - \frac{2k\mathrm{Ma}}{1-\alpha} + \frac{\alpha(2-\alpha)}{1-\alpha}\right)^{1/2} - (1 + k\mathrm{Ma})\right\}$$

+2.5

1.12 Assuming that in part 1.11 you have obtained the result

$$\sigma = \frac{k}{2-\alpha}\left\{\sqrt{1 + k^2\mathrm{Ma}^2 - \frac{2k\mathrm{Ma}}{1-\alpha} + \frac{\alpha(2-\alpha)}{(1-\alpha)}} - (1 + k\mathrm{Ma})\right\}, \tag{15}$$

for the growth rate $\sigma$, sketch $\sigma$ as a function of $k$ for fixed $\alpha = 0.5$ and for a) $\mathrm{Ma} = 0$, b) $\mathrm{Ma} = 0.2$ and c) $\mathrm{Ma} = -0.2$. According to simplified single-step chemistry analyses at large activation energies, what is the critical Lewis number $\mathrm{Le}_c$ for which Ma becomes negative? What is the impact of positive and negative Ma on flame stability?




+5

FOR $\mathrm{Ma} \le 0$ THE FLAME IS ALWAYS UNSTABLE BY HYDRODYNAMIC + DIFFUSIVE-THERMAL INSTABILITIES

IN PARTICULAR, $\mathrm{Ma} < 0$ WHEN $\mathrm{Le} < \mathrm{Le}_c = 1 - \frac{1}{\beta}\left[\frac{2}{1-\alpha}\ln\left(\frac{1}{1-\alpha}\right)\right] \Big/ \int_0^{\frac{\alpha}{1-\alpha}} \frac{\ln(1+x)}{x}\,dx$

WITH $\mathrm{Le}_c \sim 0.5$ FOR PRACTICAL APPLICATIONS

FOR $\mathrm{Ma} > 0$ THE FLAME IS HYDRODYNAMICALLY UNSTABLE AT LONG WAVELENGTHS BUT DIFFUSIVE-THERMALLY STABLE AT SHORT WAVELENGTHS, WITH $k^*$ A CUTOFF WAVENUMBER GIVEN BY $k^* = \frac{1}{2}\frac{\alpha}{\mathrm{Ma}}$.