– Course Reader – ME 471: Turbulent Combustion

(Version 2.0)

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RECOMMENDED READING

Recommended Reading

Since this course covers material from different subject areas (including aerodynamics, thermodynamics, gas turbines, and specialized topics on internal combustion engines and rocket-propulsion), we are relying on different references. Below is a list of complementary reading material for this course; all books are on reserve at the library:

- Thermodynamics:
 - Cengel & Boles: Thermodynamics: An Engineering Approach, McGraw-Hill [12];
 - Reynolds & Perkins: Engineering Thermodynamics, McGraw-Hill [55].
- Aerodynamics:
 - Anderson: Introduction to Flight, McGraw-Hill [1];
 - Anderson: Modern Compressible Flow, McGraw-Hill [2].
- Gas Turbine Engines
 - Mattingly: Elements of Propulsion: Gas Turbines and Rockets, AIAA Ed. Series. [45] (Recommended Text)
 - Saravanamuttoo, Rogers, Cohen, & Straznicky: Gas Turbine Theory, Pearson [56]
 - Hill & Peterson: Mechanics and Thermodynamics of Propulsion, Addison-Wesley [29];
 - Lefebvre: Gas Turbine Combustion, Taylor & Francis [39];
 - Farokhi: Aircraft Propulsion, Wiley [20];
 - Cumpsty: Jet Propulsion A Simple Guide to the Aerodynamic and Thermodynamic Design and Performance of Jet Engines, Cambridge University Press [16];
 - Rolls Royce: The Jet Engine A Complete Overview of the Modern Gas Turbine [62].
 - Dixon & Hall: Fluid Mechanics and Thermodynamics of Turbomachinery, Butterworth-Heinemann (also available as online resource: http://www.sciencedirect.com/science/book/9780124159549)
 - Online resource to Jane's aero engines: https://janes.ihs.com
- Internal Combustion Engines:
 - Heywood: Internal Combustion Engine Fundamentals, McGraw-Hill [28];
 - Stone: Introduction to Internal Combustion Engines, Palgrave MacMillan [60];
 - Lumley: Engines An Introduction, Cambridge University Press [41].
- Rocket Propulsion
 - Sutton & Biblarz: Rocket Propulsion Elements, Wiley [61];

 Huzel & Huang: Modern Engineering for Design of Liquid-Propellant Rocket Engines, American Institute of Aeronautics and Astronautics [30].

NOMENCLATURE

Nomenclature

Symbol	Description	Value	Units
А	Generic chemical species	-	-
A	Reaction frequency factor (order m)	-	mol^{1-m} - L^{m-1} -s
A	Area	-	m^2
D	Diameter	-	m
E_A	Activation energy	-	$\rm J/mol$
E	Internal energy	-	J
G	Distance function	-	-
H	Enthalpy	-	J
\underline{I}	Identity tensor	-	-
\overline{K}	Equilibrium constant	-	-
N	Number of a generic quantity	-	-
N	Number of molecules/atoms	-	-
Р	Probability density function	-	-
Q	Prior probability density function	-	_
õ	Heat Release	-	J
\tilde{R}	Gas constant		J/(kg-K)
R	Correlation function	-	-
S	Entropy	_	J/K
\tilde{T}	Temperature	_	K
V	Volume	_	m ³
V	Diffusion velocity of species α	_	m/s
$\frac{V}{W}^{\alpha}$	Molecular weight	_	g/mol
W	Wiener Process	_	8/ mor
X .	Mole fraction of species α	_	_
V_{-}	Mass fraction of species α	_	_
Z	Mixture fraction	_	_
Z	Compressibility		
2	Speed of sound	_	- m/s
	Specific heat capacity at constant (prossure	-	$I/(\log K)$
$c_{\{p,v\}}$	volume)	-	J/(Kg-IX)
	Specific internal energy		I /lea
ê	Unit weaton	-	J/Kg
e	Crewitational acceleration	-	- m /a ²
$\frac{g}{h}$		-	III/S
n	Diffusion from of on original	-	J/Kg
$\frac{j}{\alpha}$	Diffusion flux of species α	-	kg/m^{-s}
k	Rate constant (order m)	-	mol ¹ - <i>m</i> -L ^{<i>m</i>-1} -s
k_B	Boltzmann constant	1.3806×10^{-23}	J/K
m	Mass	-	kg
n	Number of moles	-	mol
$\underline{\hat{n}}$	Normal vector	-	-
p	Pressure	-	Pa
\underline{q}	Heat flux vector	-	W/m^3
s	Flame speed	-	m/s

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s	Specific entropy	-	J/(kg-K)
u	Velocity vector	-	m/s
\overline{v}	Specific volume	-	m^3/kg
w_{lpha}	Volumetric reaction rate of species α	-	$1/m^3-s$
y	Element mass fraction	-	-
α_{α}	Diffusivity of species α	-	m^2/s
α^T	Thermal diffusivity	-	m^2/s
χ	Scalar dissipation rate	-	1/s
δ	Dirac delta function	-	-
δ	Characteristic thickness	-	m
ϵ	Turbulent dissipation rate	-	m^2/s^3
η	Kolmogorov scale	-	m
γ	Specific heat ratio	-	-
λ	Thermal conductivity	-	W/(m-K)
λ_g	Taylor microscale	-	m
Λ	Burning rate eigenvalue	-	m/s
κ	Bulk viscosity	-	Pa-s
κ	Wavenumber	-	$,^{-1}$
ho	Density	-	$ m kg/m^3$
μ	Dynamic Viscosity	-	Pa-s
ν	Kinematic Viscosity	-	m^2/s
$ u_{lpha}, u_{lpha}', u_{lpha}''$	Stoichiometric coefficient, mole number of	-	-
	species α		
$\dot{\omega}_{lpha}$	Production rate of species α	-	1/s
ϕ	Equivalence ratio	-	-
Φ	Two-point autocorrelation function	-	-
$\underline{\sigma}$	Viscous stress tensor	-	\mathbf{Pa}
au	Timescale	-	s
ξ	Generic variable	-	-
ζ	Generic variable	-	-
ψ	Streamfunction	-	m^2/s
$\sum_{n \in \mathbb{N}}$	Flame surface density	-	-
(\cdot)	Unit vector	-	-
$\overline{(\cdot)}$	Mean quantity	-	-
$(\cdot)'$	Fluctuating quantity	-	-
$(\cdot)^0$	At reference conditions	-	-
$(\cdot)_0$	At reference conditions	-	-
$(\cdot)_a$	Activation	-	-
$(\cdot)_{f}$	Forward reaction (k)	-	-
$(\cdot)_{f}$	Formation (h)	-	-
$(\cdot)_{l}^{j}$	Reaction indicator	-	-
$(\cdot)_t$	Turbulent	-	-
(\cdot)	Generic vector	-	-
$\overline{(\cdot)}$	Generic tensor	-	-
$\overline{(\cdot)}$	Rate (time derivative)	-	1/s
$\widetilde{(\cdot)}$	Favre average	-	-

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NOMENCLATURE

$\langle \cdot \rangle$	Ensemble average	-	-
$(\cdot)_{\rm F}$	Fuel stream	-	-
$(\cdot)_{I}$	Jet	-	-
$(\cdot)_L$	Laminar	-	-
$(\cdot)_{0}$	Oxidizer stream	-	-
$(\cdot)_{\mathbf{P}}$	Products	-	-
$(\cdot)_{R}$	Radiation	-	-
$(\cdot)_{st}$	Stoichiometric conditions	-	-
$(\cdot)_b$	Burned gas (u)	-	-
$(\cdot)_b$	Reverse reaction (k)	-	-
$(\cdot)_s$	Sensible (h) ;	-	-
$(\cdot)_s$	Species (N)	-	-
$(\cdot)_m$	Molar	-	-
$(\cdot)_t$	Time (∂)	-	-
$(\cdot)_t$	$\mathrm{Total}(h);$	-	-
$(\cdot)_u$	Unburned gas	-	-
$(\cdot)_{\alpha}$	Species indicator	-	-
$(\cdot)_{\beta}$	Species indicator	-	-
\mathcal{F}	Fuel	-	-
${\cal H}$	Heaviside function	-	-
\mathcal{L}	General transport operator	-	-
\mathcal{M}	Markstein Length	-	m
\mathcal{O}	Oxidizer	-	-
\mathcal{U}	Velocity sample space variable	-	-
${\mathcal Y}$	Mass fraction sample space variable	-	-
\mathcal{R}	Universal gas constant	8.314	J/(mol K)
Re	Reynolds number	-	-
Ce	Heat release parameter	-	-
Da	Damköhler number	-	-
Ec	Eckhart number	-	-
Fr	Froude number	-	-
Le	Lewis number	-	-
M	Mach number	-	-
Sc	Schmidt number	-	-
Ze	Zeldovich number	-	-

CHAPTER 1

Course Information

1.1. Course Organization

The goal of this course is to integrate concepts from turbulence, combustion, and mathematics to give the reader a thorough understanding of turbulent combustion. To accomplish this, the course has the following outline:

- (1) Governing Equations
 - Key definitions
 - Conservation equations
 - Transport models
 - Chemical models
 - State equations
- (2) Mathematical Analysis of Simple Flames
 - Nondimensionalization
 - Important modeling simplifications
- (3) Review of Mathematical and Combustion-Physical Concepts
 - Turbulence: filtering, averaging, statistical analysis
 - Combustion: premixed and non-premixed
- (4) Combustion Modeling
 - Topology-based combustion modelling
 - Topology-free combustion models
 - Pollutants and emissions
 - Combustion instabilities
 - Spray combustion
- (5) Selected topics
 - RANS
 - LES
 - DNS
 - Heterogeneous combustion
 - Plasma-assisted combustion
 - Flame stabilization

1. COURSE INFORMATION

1.2. Computing Environment

During the course of this class, it will be instructive to utilize the Cantera software package to compute a variety of quantities relevant to turbulent combustion. It is highly recommended that this package be installed within the Anaconda python distribution to ensure cross-platform operability as well as consistency in results, syntax, and debugging. Steps to install and test are as follows:

- (1) Download and install the latest version of the Anaconda python distribution.
- (2) Execute the following command to install Cantera and other dependencies within a virtual environment called "canpy" running Python 2.7.
 conda create -n canpy -c cantera cantera ipython matplotlib jupyter python=2.7
- (3) You can now activate this environment at any point by running,

source activate canpy or deactivate by running,

source deactivate

(4) Additional instructions on installing Cantera can be found here.

Once Cantera has installed successfully, you can test package operability by executing a simple premixed flame calculation in the Jupyter notebook provided in Sec. 8.1. Execute the command,

jupyter notebook

select "Notebook" from under the "New" menu, and you will be presented with a blank notebook. You can then insert the provided code, which will import the Cantera package, define several useful functions for interacting with the solution object, print gas parameters, and plot the structure of a stoichiometric premixed flame. Additional documentation can be found on the Cantera website.

CHAPTER 2

Definitions and Governing Equations

Chemically reacting flows are fully described by conservation equations for mass, momentum, species, and energy with the state equation relating thermodynamic properties to one another. In the following, we present key definitions, introduce important combustion concepts, and define governing equations together with constitutive relations that form the foundation of combustion science.

2.1. General Definitions

2.1.1. Equation of State. An equation of state defines a constitutive relation between two or more thermodynamic variables. The most common form is the ideal gas law. The ideal gas law can be expressed in different, but equivalent forms, as:

Mass-specific:
$$pV = mRT$$
, (2.11)

Mole-specific:
$$pV = n\mathcal{R}T$$
, (2.12)

Molecule/atom-specific:
$$pV = Nk_BT$$
, (2.13)

where \mathcal{R} is the universal gas constant, and $R = \mathcal{R}/W$ is the gas constant of the mixture.

The ideal gas law, Eqs. (2.11)-(2.13), is applicable for conditions such that the distance between molecules is sufficiently large and no intermolecular forces exists between molecules. As an example of a situation wherein this equation of state would not apply, consider the case of rocket combustion, where high-pressure fuel injection requires consideration of realfluid effects. A common form for these real-fluid state equations is the cubic state equation,

$$p = \frac{RT}{v-b} - \frac{\Theta(v-\eta)}{(v-b)(v^2 + \delta v + \epsilon)},$$
(2.14)

where $\Theta, b, \eta, \epsilon$, and δ are parameters depending on temperature, mixture, and critical conditions [51]. To evaluate the deviation from the ideal-gas conditions, the *compressibility* Z is commonly introduced:

$$\mathcal{Z} = \frac{pV}{mRT}.$$
(2.15)

2. DEFINITIONS AND GOVERNING EQUATIONS



FIGURE 2.11 Thermodynamic state plane and supercritical state structure. The Widom line is an extension to the coexistence line at critical pressure, and marks the crossover between supercritical liquidlike and gaslike states. The dashed line where the compressibility Z = 0.95 denotes the transition to an ideal gas.

where $\mathcal{Z} = 1$ denotes an ideal gas, and conditions for $\mathcal{Z} > 1$ or $\mathcal{Z} < 1$ require the consideration of real-fluid effects. The region where the ideal gas law is approximately valid is shown in Fig. 2.11. Often, the real-fluid state equations are explicitly written in terms of \mathcal{Z} .

2.1.2. Mass Fraction and Mole Fraction. We can define the mass fraction of species α , Y_{α} as,

$$Y_{\alpha} = \frac{\rho_{\alpha}}{\rho} = \frac{m_{\alpha}}{m},\tag{2.16}$$

where $m = \sum_{\alpha=1}^{N_s} m_{\alpha}$ is the total mass of the species.

The mole fraction of species α , X_{α} , is defined as,

$$X_{\alpha} = \frac{n_{\alpha}}{n},\tag{2.17}$$

2.1. GENERAL DEFINITIONS

where $n = \sum_{\alpha=1}^{N_s} n_{\alpha}$ is the number of moles of all species. Conservation of mass and conservation of moles require that,

$$\sum_{\alpha=1}^{N_s} Y_{\alpha} = \sum_{\alpha=1}^{N_s} X_{\alpha} = 1.$$
 (2.18)

By using the ideal gas law from Eq. (2.12), we can define the partial pressure p_{α} of species α as,

$$p_{\alpha}V = n_{\alpha}\mathcal{R}T. \tag{2.19}$$

By taking the ratio between Eq. (2.19) and Eq. (2.12), we obtain

$$\frac{p_{\alpha}}{p} = \frac{n_{\alpha}}{n} \to p_{\alpha} = X_{\alpha}p, \qquad (2.110)$$

which is Dalton's Law. Dalton's law of partial pressure can be expressed in both mole-based and mass-based forms,

$$p = \sum_{\alpha=1}^{N_s} p_\alpha = \sum_{\alpha=1}^{N_s} X_\alpha p \qquad \text{(Mole-specific)} \tag{2.111a}$$

$$\rho = \sum_{\alpha=1}^{N_s} \rho_\alpha = \sum_{\alpha=1}^{N_s} Y_\alpha \rho \qquad \text{(Mass-specific)}.$$
 (2.111b)

We can also write the mass of a particular species as,

$$m_{\alpha} = n_{\alpha} W_{\alpha}, \tag{2.112}$$

and the mean molar mass W can be expanded as,

$$\frac{1}{W} = \frac{1}{W} \sum_{\alpha=1}^{N_s} \frac{n_\alpha}{n} = \sum_{\alpha=1}^{N_s} \frac{n_\alpha W_\alpha}{nW} \frac{1}{W_\alpha} = \sum_{\alpha=1}^{N_s} \frac{m_\alpha}{m} \frac{1}{W_\alpha} = \sum_{\alpha=1}^{N_s} \frac{Y_\alpha}{W_\alpha}.$$
 (2.113)

Using this result, we can relate the mass fraction and mole fraction via the mixture molar mass,

$$W = \sum_{\alpha=1}^{N_s} X_{\alpha} W_{\alpha} = \left(\sum_{\alpha=1}^{N_s} \frac{Y_{\alpha}}{W_{\alpha}}\right)^{-1}.$$
 (2.114)

Further, some simple algebra using Eq. (2.112) relates the mass and mole fractions,

$$X_{\alpha} = \frac{n_{\alpha}}{n} = \frac{m_{\alpha}/W_{\alpha}}{\sum_{\alpha=1}^{N_s} m_{\alpha}/W_{\alpha}} = \frac{Y_{\alpha}/W_{\alpha}}{\sum_{\alpha=1}^{N_s} Y_{\alpha}/W_{\alpha}} = \frac{WY_{\alpha}}{W_{\alpha}}.$$
 (2.115)

The ability to relate mass and mole fractions can become quite useful in intuitively expressing the results of much of the analysis we will present.

2.2. Stoichiometry and Equivalence Ratio

The generic form of a chemical reaction can be written as

$$\sum_{\alpha=1}^{N_s} \nu'_{\alpha} \mathbf{A}_{\alpha} \rightleftharpoons \sum_{\alpha=1}^{N_s} \nu''_{\alpha} \mathbf{A}_{\alpha}, \qquad (2.21)$$

with A_{α} denoting the chemical species α , ν' and ν'' the stoichiometric coefficients for reactants and products, and $\nu_{\alpha} = \nu''_{\alpha} - \nu'_{\alpha}$ the net stoichiometric coefficient. In this context, we would like to emphasize the difference between the stoichiometric coefficient (ν', ν'') and mole number (n): While the stoichiometric coefficient is determined by the law of mass action through a chemical conversion reaction, the mole-number is a local quantity that can change depending on flow-field conditions. Only for the condition that $n_{\alpha} = n_{\alpha}$, st, that is stoichiometric conditions, are both quantities identical.

We can now consider a generic stoichiometric reaction of fuel F and oxidizer O forming a product P,

$$\nu_{\rm F}' \mathbf{F} + \nu_{\rm O}' \mathbf{O} \rightleftharpoons \nu_{\rm P} \mathbf{P},\tag{2.22}$$

by defining the mole ratio, which is equal to the ratio of stoichiometric coefficients in the unburned mixture (denoted with subscript "u"). With Eq. (2.112), it follows that,

$$\frac{n_{\mathrm{O},u}}{n_{\mathrm{F},u}}\Big|_{\mathrm{st}} = \frac{X_{\mathrm{O},u}}{X_{\mathrm{F},u}}\Big|_{\mathrm{st}} = \frac{\nu'_{\mathrm{O}}}{\nu'_{\mathrm{F}}}$$
(2.23)

$$\frac{m_{\mathrm{O},u}}{m_{\mathrm{F},u}}\bigg|_{\mathrm{st}} = \frac{Y_{\mathrm{O},u}}{Y_{\mathrm{F},u}}\bigg|_{\mathrm{st}} = \frac{\nu'_{\mathrm{O}}W_{\mathrm{O}}}{\nu'_{\mathrm{F}}W_{\mathrm{F}}} \equiv \nu, \qquad (2.24)$$

where ν is the stoichiometric fuel-air ratio. From these definitions, we can derive the equivalence ratio, which is the standard quantity defining the relative amounts of fuel and oxidizer in a reacting flow,

$$\phi = \frac{m_{\rm F}/m_{\rm O}}{(m_{\rm F}/m_{\rm O})_{\rm st}} = \frac{Y_{\rm F,u}/Y_{\rm O,u}}{(Y_{\rm F,u}/Y_{\rm O,u})_{\rm st}} = \nu \frac{Y_{\rm F,u}}{Y_{\rm O,u}}.$$
(2.25)

More commonly, we consider the equivalence ratio ϕ , which is defined with respect to the fuel and air mixture,

$$\phi = \frac{m_{\rm F}/m_{\rm air}}{(m_{\rm F}/m_{\rm air})_{\rm st}}.$$
(2.26)

2.3. MIXTURE FRACTION

Note that the ranges of ϕ are as follows,

$$\phi \begin{cases} < 1 & \text{Fuel lean} \\ = 1 & \text{Stoichiometric} \\ > 1 & \text{Fuel rich} \end{cases}$$
(2.27)

2.3. Mixture Fraction



FIGURE 2.31 Schematic of a two-stream combustion chamber.

The mixture fraction Z describes the local equivalence ratio in the mixture. This quantity physically describes the amount of local mixture that originated from the fuel stream, and is introduced as a non-dimensional quantity with the specific purpose of describing non-premixed flames via a conserved scalar. Consider a two-stream non-premixed burner system in which the fuel is injected through stream \mathcal{F} and the oxidizer is injected through stream \mathcal{O} as in Fig. 2.31,

Fuel + Oxidizer
$$\rightarrow$$
 Products
 $m_{\rm F}F + m_{\rm O}O \rightarrow (m_{\rm F} + m_{\rm O})P$ (R1)

1kg F +
$$\left(\frac{m_{\rm O}}{m_{\rm F}}\right)_{\rm st}$$
 O $\rightharpoonup \left(1 + \left(\frac{m_{\rm O}}{m_{\rm F}}\right)_{\rm st}\right)$ P, (R2)

For this twos-stream system, we can define the coupling function ξ

$$\xi = \nu Y_{\rm F} - Y_{\rm O} , \qquad (2.32)$$

which measures the deviation from the local stoichiometric. From this, we can introduce the mixture fraction Z,

$$Z = \frac{\xi^* - \xi_{\rm O}}{\xi_{\rm F} - \xi_{\rm O}}; \quad Z \in [0, 1].$$
(2.33)

which provides a normalization so that $Z = 0(\xi^* \to \xi_{\rm O})$ defines the condition in the oxidizer stream and $Z = 1(\xi^* \to \xi_{\rm F})$ defines the condition in the fuel stream. Qualitatively, the mixture fraction can be considered as quantity that represents that normalized mass of material originating from the fuel stream.



FIGURE 2.32 Diffusion flame representation in both unburned and burned states.

We can now consider the simplified case where only fuel or oxidizer are present in the fuel (stream \mathcal{F}) and oxidizer (stream \mathcal{O}) streams, meaning that $Y_{O,\mathcal{F}} = Y_{F,\mathcal{O}} = 0$. This situation simplifies the expression of the mixture fraction to,

$$Z = \frac{(\nu Y_{\rm F} - Y_{\rm O})^* + Y_{\rm O,\mathcal{O}}}{\nu Y_{\rm F,\mathcal{F}} + Y_{\rm O,\mathcal{O}}}.$$
(2.34)

By considering a stoichiometric mixture such that $\nu Y_{\rm F} = Y_{\rm O}$, we have,

$$Z_{st} = \frac{Y_{\mathcal{O},\mathcal{O}}}{\nu Y_{\mathcal{F},\mathcal{F}} + Y_{\mathcal{O},\mathcal{O}}} = \left[1 + \frac{\nu Y_{\mathcal{F},\mathcal{F}}}{Y_{\mathcal{O},\mathcal{O}}}\right]^{-1}.$$
(2.35)

As a brief clarification, consider the reaction:

$$\nu'_{\rm F} \mathbf{F} + \nu'_{\rm O} \mathbf{O} \rightharpoonup \nu''_{\rm P} \mathbf{P} = (\nu'_{\rm F} + \nu'_{\rm O}) \mathbf{P} \tag{R3}$$

$$\nu_{\rm F}' W_{\rm F} F + \nu_{\rm O}' W_{\rm O} O \rightharpoonup \nu_{\rm P}'' W_{\rm P} P = (m_{\rm F} + m_{\rm O}) P. \tag{R4}$$

From this formulation, an expression relating the equivalence ratio ϕ to the mixture fraction can be obtained. We can first rewrite Eq. (2.33) as,

$$Z = \frac{(\nu Y_{\rm F} - Y_{\rm O})_u + Y_{\rm O,\mathcal{O}}}{\nu Y_{\rm F,\mathcal{F}} + Y_{\rm O,\mathcal{O}}} = \frac{(\nu Y_{\rm F} - Y_{\rm O})_u}{\nu Y_{\rm F,\mathcal{F}} + Y_{\rm O,\mathcal{O}}} + \frac{Y_{\rm O,\mathcal{O}}}{\nu Y_{\rm F,\mathcal{F}} + Y_{\rm O,\mathcal{O}}}$$
(2.36)

Now, using Eq. (2.25) and the fact that $Y_{F,u} = Y_{F,\mathcal{F}}Z$ and $Y_{O,u} = Y_{O,\mathcal{O}}(1-Z)$ as in Fig. 2.32, we can write the mixture fraction as,

$$Z = Z_{st}(1-Z)(\phi-1) + Z_{st}, \qquad (2.37)$$

2.3. MIXTURE FRACTION

and solve for ϕ as,

$$\phi = \frac{Z}{1-Z} \frac{1-Z_{st}}{Z_{st}}.$$
(2.38)

We now present a few remarks on the mixture fraction:

- Key requirements:
 - Derived from linear combination of subset of species mass fractions
 - Conserved property (i.e. no scalar source term)
 - Bounded between $Z \in [0,1]$ ($Z \to 0$ for oxidizer stream, $Z \to 1$ for fuel stream)
 - Representation of local composition with respect to fuel stream composition
- The definition that we introduced was based on a one-step global chemical reaction, and the combination of fuel/oxidizer mass fraction ($\nu Y_{\rm F} - Y_{\rm O}$) was selected so as to eliminate the source term from the corresponding species equation. Analysis demonstrating this point in more detail will be discussed in Sec. 3.3.
- An extension of the mixture fraction to multistep reactions can be facilitated by considering the elemental mass fraction, which was first introduced by [5]. Such an expression involves relating mixture fraction to the elemental mass fractions of carbon, hydrogen, and oxygen. In the case of carbon, for instance,

$$y_C = \sum_{\alpha=1}^{N_s} n_{C,\alpha} \frac{Y_{\alpha} M_C}{M_{\alpha}}, \qquad (2.39)$$

where $n_{C,\alpha}$ is the number of carbon atoms in species α . A main issue with this definition is the difficulty in writing a conservation equation that is mathematically tractable.

- The mixture fraction formulation presented within this section is limited to twostream systems. Extensions to multi-stream systems can be enabled via use of a barycentric coordinate system or an elemental formulation, as discussed in Discussion Box 1.
- Extending the mixture fraction concept to liquid/gas-phase systems such as spray flames can be accomplished in effective composition space, as detailed in Discussion Box 2.

Discussion Box 1: Various Elemental Mixture Fractions

The appropriate definition of the mixture fraction is heavily dependent on the particular problem at hand. In [16] and [16], for instance, a piloted premixed jet flame is simulated, which requires differentiating between the compositions in the pilot and coflow oxidizer streams. Thus, the mixture fraction definition used is,

$$\underline{\underline{A}} = \begin{pmatrix} y_C^{\rm F} - y_C^{\rm O(0)} & y_C^{\rm O(1)} - y_C^{\rm O(0)} \\ y_H - y_H^{\rm O(0)} & y_H^{\rm O(1)} - y_H^{\rm O(0)} \end{pmatrix}, \quad \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix} = \underline{\underline{A}}^{-1} \begin{pmatrix} y_C - y_C^{\rm O(0)} \\ y_H - y_H^{\rm O(0)} \end{pmatrix}$$
(2.310)

The work of [46] and [46], on the other hand, consider a burner with both a coflow and an air shroud, which requires a slightly different formulation. The important point here is that the system configuration often determines the best mathematical modeling formulation!

Discussion Box 2: Generalizing the Mixture Fraction: Spray Diffusion Flames

Fundamentally, the classical mixture-fraction formulation cannot be used in spray flames wherein liquid fuels are combusted because this expression becomes non-monotonic as a result of an evaporation source term in the corresponding conservation equations. The effective composition space can be defined as $d\eta$, and combines the mixture fraction defined for the gaseous phase, Z_g , and the mixture fraction of the liquid phase, Z_l . It is shown by [33] that this quantity $d\eta = \sqrt{(dZ_g)^2 + (dZ_l)^2}$, which reduces to classical mixture fraction Z_g for gaseous systems, can utilize the liquid-to-gas mass ratio Z_l to correctly predict the behavior of laminar, one-dimensional counterflow spray flames.

2.4. Enthalpy, Internal Energy, and Thermodynamic Properties

In combustion, we are mostly concerned with control volume analysis, so it is usually convenient to work with enthalpy. We define the specific *sensible* + *chemical enthalpy* of species α as,

$$dh_{\alpha} = c_p dT + h_{f,\alpha}^0 \tag{2.41}$$

$$h_{\alpha} = \underbrace{\int_{T_0}^T c_{p,\alpha} dT}_{h_s} + \underbrace{h_{f,\alpha}^0}_{h_c}, \tag{2.42}$$

where the first term is the sensible enthalpy and the second term is the chemical enthalpy. The enthalpy of a mixture can then be written in terms of the total sensible and chemical enthalpies,

$$dh = h_{\alpha}dY_{\alpha} + dh_{\alpha}Y_{\alpha} \tag{2.43}$$

$$h = \sum_{\alpha=1}^{N_s} h_{\alpha} Y_{\alpha} = \int_{T_0}^{T} c_p dT + \sum_{\alpha} h_{f,\alpha}^0 Y_{\alpha}, \qquad (2.44)$$

2.5. CONSERVATION EQUATIONS

where $c_p = \sum_{\alpha=1}^{N_s} Y_{\alpha} c_{p,\alpha}$ is the specific heat capacity of the mixture at constant pressure. We can similarly define the specific *total enthalpy* as the sum of the mixture enthalpy and the kinetic energy as,

$$h_t = \int_{T_0}^T c_p dT + \sum_{\alpha=1}^{N_s} h_{f,\alpha}^0 Y_\alpha + \frac{1}{2} |\underline{u}|^2, \qquad (2.45)$$

where the last term is the specific kinetic energy. In differential form, this can be written

$$dh_t = c_p dT + \sum_{\alpha=1}^{N_s} h_{f,\alpha}^0 dY_\alpha + u_i du_i.$$
(2.46)

Finally, the following relation defines the internal energy e in terms of the sensible enthalpy, pressure, and density,

$$de = dh - d(p/\rho), \tag{2.47}$$

such that,

$$e = \int_{T_0}^T c_v dT - RT_0 + \sum_{\alpha=1}^{N_s} h_{f,\alpha}^0 Y_\alpha.$$
 (2.48)

We also note that the specific heat capacities at constant volume (c_v) and constant pressure (c_p) are related by the ratio of specific heat, γ ,

$$\gamma = \frac{c_p}{c_v}.\tag{2.49}$$

Note that the specific heats for various quantities have been tabulated for both high and low temperature regimes. These can generally be found in the form of NASA polynomials [10],

$$c_{p,v} = \sum_{i=-2}^{5} a_i T^i.$$
(2.410)

2.5. Conservation Equations

Chemically reacting flows are described by the conservation equations for mass, momentum, energy, and species. Here we derive these equations in general form and introduce simplifications that are often used for turbulent flow simulation. **2.5.1. Continuity Equation.** The continuity equation, which describes conservation of mass, can be written with full generality as follows:

$$\partial_t \rho + \nabla \cdot (\rho \underline{u}) = 0, \qquad (2.51)$$

where ρ is the density and <u>u</u> is the velocity vector. By introducing the substantive derivative,

$$D_t \equiv \partial_t + \underline{u} \cdot \nabla, \tag{2.52}$$

we can express Eq. (2.51) as,

$$D_t \rho = -\rho \nabla \cdot \underline{u},\tag{2.53}$$

which represents the net change of volume following a control mass. From this, it follows for a generic scalar quantity that,

$$\partial_t(\rho\phi) + \nabla \cdot (\rho\phi\underline{u}) = \rho\partial_t\phi + \phi\partial_t\rho + \rho\underline{u} \cdot \nabla\phi + \phi\nabla \cdot (\rho\underline{u})$$
(2.54a)

$$= \rho(\partial_t \phi + \underline{u} \cdot \nabla \phi) + \phi(\partial_t \rho + \nabla \cdot (\rho \underline{u}))$$
(2.54b)

$$=\rho D_t \phi \tag{2.54c}$$

2.5.2. Momentum Conservation. The momentum conservation equation can be written as,

$$\rho D_t \underline{u} = \partial_t (\rho \underline{u}) + \nabla \cdot (\rho \underline{u} \otimes \underline{u}) = -\nabla p + \nabla \cdot \underline{\underline{\sigma}} + \sum_{\alpha=1}^{N_s} \rho Y_\alpha \underline{g_\alpha}, \qquad (2.55)$$

where \underline{g}_{α} denotes the vector of body forces acting on species α and $\underline{\sigma}$ is the viscous stress tensor.

2.5.3. Species Conservation. It is most convenient to consider species conservation in terms of the mass fraction of species α ,

$$\rho D_t Y_\alpha = \partial_t (\rho Y_\alpha) + \nabla \cdot (\rho \underline{u} Y_\alpha) = -\nabla \cdot \underline{j_\alpha} + \rho \dot{\omega}_\alpha, \qquad (2.56)$$

where $\underline{j_{\alpha}}$ is the species diffusion flux and $\rho \dot{\omega}_{\alpha}$ is the chemical source term of species α . The species diffusion flux in Eq. (2.56) can be expressed as,

$$\underline{j_{\alpha}} = -\rho \underline{V_{\alpha}} Y_{\alpha}, \qquad (2.57)$$

with \underline{V}_{α} the diffusion velocity of species α . We will consider models for this quantity in Sec. 2.6.2. By considering Eq. (2.111b) and the relation between species conservation

Eq. (2.56) and mass conservation Eq. (2.51), we can observe that the following relation must hold,

$$\sum_{\alpha=1}^{N_s} \left[\partial_t(\rho Y_\alpha) + \nabla \cdot (\rho \underline{u} Y_\alpha)\right] = \partial_t \rho + \nabla \cdot (\rho \underline{u}) \equiv 0.$$
(2.58)

In light of Eq. (2.56), this directly implies the following constraints

$$\sum_{\alpha=1}^{N_s} \nabla \cdot \underline{j_\alpha} = 0 \tag{2.59}$$

$$\sum_{\alpha=1}^{N_s} \rho \dot{\omega}_{\alpha} = 0. \tag{2.510}$$

2.5.4. Total Enthalpy Conservation. For open combustion systems it is convenient to express energy conservation in terms of total enthalpy. Recalling Eq. (2.46), we can express conservation of enthalpy as follows,

$$\rho D_t h_t = \partial_t (\rho h_t) + \nabla \cdot (\rho \underline{u} h_t) = \partial_t p - \nabla \cdot q + \nabla \cdot (\underline{\sigma} \cdot \underline{u}) + \rho \sum_{\alpha=1}^{N_s} Y_\alpha \underline{g_\alpha} \cdot (\underline{u} + \underline{V_\alpha}), \quad (2.511)$$

where $\partial_t p$ is the pressure work, $-\nabla \cdot q$ is the heat flux, $\nabla \cdot (\underline{\sigma} \cdot \underline{u})$ is the viscous dissipation, and $\rho \sum_{\alpha=1}^{N_s} Y_{\alpha} \underline{g_{\alpha}} \cdot (\underline{u} + \underline{V_{\alpha}})$ is the external body force work. By subtracting the rate of change of the kinetic energy, we obtain an expression for the sensible and chemical enthalpy,

$$\partial_t(\rho h) + \nabla \cdot (\rho \underline{u} h) = D_t p - \nabla \cdot q + \underline{\underline{\sigma}} : \nabla \underline{\underline{u}} + \rho \sum_{\alpha=1}^{N_s} Y_\alpha \underline{\underline{g}}_\alpha \cdot \underline{V}_\alpha.$$
(2.512)

Using Eq. (2.48), the conservation equation for the chemical and sensible internal energy can be written as,

$$\rho D_t e = \partial_t (\rho e) + \nabla \cdot (\rho \underline{u} e) = -\nabla \cdot q + \underline{\sigma} : \nabla \underline{u} - p \nabla \cdot \underline{u} + \rho \sum_{\alpha=1}^{N_s} Y_\alpha \underline{g_\alpha} \cdot \underline{V_\alpha}, \qquad (2.513)$$

where $\underline{\sigma}: \nabla \underline{u}$ is the viscous dissipation and $p \nabla \cdot \underline{u}$ is the pressure-dilatation work.

2.6. Constitutive Relations and Transport Properties

We can now complete the conservation equations by prescribing the constitutive relations for viscous stress and diffusive flux of both heat and mass. **2.6.1.** Viscous Stress Tensor. Here, we consider only Newtonian fluids, meaning that viscosity is only a function of fluid properties (\underline{Y},T) , but not dependent on the strain rate or local velocity field. For this, we can write the viscous stress tensor in the following form,

$$\underline{\underline{\sigma}} = \mu [\nabla \underline{\underline{u}} + (\nabla \underline{\underline{u}})^T] + \lambda \nabla \cdot \underline{\underline{u}} \, \underline{\underline{I}}, \tag{2.61}$$

where μ is the dynamic viscosity, $\nu = \mu/\rho$ is the kinematic viscosity, $\lambda = \kappa - 2\mu/3$ is the second viscosity coefficient, and κ is the dilatational (or bulk) viscosity coefficient; κ describes the irreversible conversion of mechanical work into heat by dilatational strain (sound waves, ultrasonic waves, etc.). The contribution of the dilatational viscous flux $(\kappa\nabla \cdot \underline{u})$ is small in dilute monatomic gases, low-Mach flows $(\nabla \cdot \underline{u} \to 0)$, or boundary layers. However, the ratio of κ/μ becomes significant for species relevant for combustion applications (H₂ ~ 20, CH₄ ~ 2, O₂ ~ 1, N₂ ~ 1). The effect of bulk viscosity (see Discussion Box 3) also requires consideration in high speed flows; this is seldom done, as the effects of κ/μ are commonly neglected in flows of engineering interest. For more information on this subject, see [24]. Finally, note that with $\kappa = 0$, we obtain the common form of the viscous stress tensor,

$$\underline{\underline{\sigma}} = \mu [\nabla \underline{\underline{u}} + (\nabla \underline{\underline{u}})^T] - \frac{2}{3} \mu \nabla \cdot \underline{\underline{uI}}$$
(2.62)

Discussion Box 3: History and Impact of Bulk Viscosity on Combustion Systems.

Stokes, Saint-Venant, and others originally made an argument that the bulk viscosity κ could be set to zero in flows of practical interest – in fact, over the years this assumption has become known as Stokes' hypothesis. Indeed, this idea was supported by the fact that both kinetic theory and experiment predict $\kappa = 0$ for a dilute monatomic gas. The $\kappa = 0$ assumption, however, is effectively equivalent to stating that dilatational effects for a given problem can be neglected. Recent studies using Direct Numerical Simulation (DNS) have shown that this assumption is not valid in many flows of engineering interest [26].

In particular, in the context of combustion, it has recently been shown through DNS that the effect of bulk viscosity can be important, but highly problem-dependent. Laminar flames, for instance, are not modified by bulk viscosity, while the local structure and global properties of turbulent flames may differ considerably when taking bulk viscous effects into account [21]. While the modifications induced by the bulk viscosity transport term are extremely small at first, they are indeed sufficient to lead to completely different realizations at a later time due to the chaotic nature of turbulence. Interestingly, this work has also shown a distinct fuel-sensitivity of bulk viscosity effect. While the inclusion of bulk viscosity is highly recommended for DNS calculations using hydrogen-containing fuels, the effects of these terms are often negligible in flames involving high-hydrocarbon fuels.

It is at this point also important to consider the dependency of viscosity on mixture composition and temperature – several different approximations are employed, each of which has a different scaling with temperature of the form,

$$\frac{\nu}{\nu_0} \sim \left(\frac{T}{T_0}\right)^m,\tag{2.63}$$

with,

$$\nu = \mu/\rho, \tag{2.64}$$

the kinematic viscosity. Several common approximations are as follows:

(1) Chapman-Approximation:

$$\mu = \mu_0 \left(\frac{T}{T_0}\right),\tag{2.65}$$

with μ_0 , T_0 reference quantities. In terms of the kinematic viscosity, this yields the following scaling,

$$\frac{\nu}{\nu_0} = \frac{\mu}{\mu_0} \frac{\rho_o}{\rho} \neq f(T).$$
(2.66)

(2) <u>Sutherland Form</u>:

$$\mu = \mu_0 \frac{T_0 + T_s}{T + T_s} \left(\frac{T}{T_0}\right)^{3/2},$$
(2.67)

with the Sutherland temperature $T_s \approx 110.4$ K. In this case, we observe a non-trivial scaling with temperature,

$$\frac{\nu}{\nu_0} = \frac{\mu}{\mu_0} \frac{\rho_0}{\rho} = \frac{T_0 + T_s}{T + T_s} \left(\frac{T}{T_0}\right)^{1/2}.$$
(2.68)

(3) <u>Wilke Form</u>:

$$\mu = \sum_{\alpha=1}^{N_s} \frac{X_{\alpha} \mu_{\alpha}}{\sum_{\beta=1}^{N_s} X_{\beta} \Phi_{\alpha\beta}},\tag{2.69}$$

where
$$\Phi_{\alpha\beta} = \frac{1}{\sqrt{8}} \left(1 + \frac{W_{\alpha}}{W_{\beta}} \right)^{-1/2} \left[1 + \left(\frac{\mu_{\alpha}}{\mu_{\beta}} \right)^{1/2} \left(\frac{W_{\beta}}{W_{\alpha}} \right)^{1/4} \right],$$
 (2.610)

is a function of molecular weight and viscosity of the different species and Φ is the appropriate collision cross-section. For a relevant discussion of how different approximations of the viscosity can affect combustion simulations, see [58]. Note that viscosity is generally only important in low Reynolds number flows. **2.6.2.** Species Transport. The species flux j_{α} in Eq. (2.57) introduces the diffusion velocity. There are two major approaches to computing the diffusion velocity: multi-component transport and mixture-averaged transport. In the case of full multi-component diffusion, we can write the diffusion velocity as,

$$\underline{V_{\alpha}} = -\frac{1}{X_{\alpha}W} \sum_{\beta \neq \alpha}^{N_s} W_{\beta} \alpha_{\alpha,\beta} \underline{d}_{\beta} - \frac{\alpha_{\alpha}^T}{\rho Y_{\alpha}} \nabla \ln T, \qquad (2.611)$$

where $\alpha_{\alpha,\beta}$ is the multicomponent diffusion coefficient of species α diffusing into species β , α_{α}^{T} is the thermal diffusion coefficient, and the term $\frac{\alpha_{\alpha}^{T}}{\rho Y_{\alpha}} \nabla \ln T$ describes the Soret effect, wherein the species diffusion occurs due to a temperature gradient. The diffusion vector \underline{d}_{β} can be written as,

$$\underline{d}_{\beta} = \nabla X_{\beta} + (X_{\beta} - Y_{\beta}) \nabla \ln p + \frac{\rho}{p} \sum_{\alpha=1}^{N_s} Y_{\alpha} Y_{\beta} (\underline{g_{\alpha}} - \underline{g_{\beta}}).$$
(2.612)

Note that the term ∇X_{β} describes the species gradient while the term $(X_{\beta} - Y_{\beta})\nabla \ln p$ describes diffusion flux due to a pressure gradient.

In a mixture-averaged approach, we write the diffusion velocity as the following using the Hirschfelder-Curtiss approximation,

$$\underline{V_{\alpha}} = -\frac{1}{X_{\alpha}} \alpha_{\alpha} \underline{d}_{\alpha} - \frac{\alpha_{\alpha}^{T}}{\rho Y_{\alpha}} \nabla \ln T, \qquad (2.613)$$

with α_{α} the mixture-averaged diffusion coefficient of species α defined as,

$$\alpha_{\alpha} = \frac{1 - Y_{\alpha}}{\sum_{\beta \neq \alpha}^{N_s} \frac{X_{\beta}}{\alpha_{\alpha,\beta}}}.$$
(2.614)

More detail on this formulation can be found in [50].

- Common simplifications of these species expressions include:
 - Species diffusion by temperature gradients are small (neglect thermal diffusion),

$$\underline{V_{\alpha}} = -\frac{1}{X_{\alpha}} \alpha_{\alpha} \underline{d}_{\alpha} \tag{2.615}$$

• Species diffusion by pressure gradients are small (in such situations as open flames and deflagrations). This case results in a simplified form of the diffusion velocity expression, known as Hirschfelder's Law [50],

$$\underline{V_{\alpha}} = -\alpha_{\alpha} \nabla \ln X_{\alpha}, \qquad (2.616)$$

with $\underline{d}_{\alpha} = \nabla X_{\alpha}$ from Eq. (2.612)

• Under even stronger assumptions including equal species diffusivities ($\alpha_{\alpha} = \alpha$) or binary mixtures, Fick's Law can also be used exactly,

$$\underline{V_{\alpha}} = -\alpha \nabla \ln Y_{\alpha} \tag{2.617}$$

2.6.3. Energy/Heat Flux. The heat flux vector has the following form,

$$\underline{q} = -\lambda \nabla T + \rho \sum_{\alpha=1}^{N_s} Y_{\alpha} \underline{V_{\alpha}} h_{\alpha} - \frac{p}{\rho} \sum_{\alpha=1}^{N_s} \frac{1}{Y_{\alpha}} \alpha_{\alpha}^T \underline{d}_{\alpha} + \underline{q}_R, \qquad (2.618)$$

where $\underline{q_R}$ is the radiative heat flux, $\lambda \nabla T$ is the conductive heat flux, $\rho \sum_{\alpha=1}^{N_s} Y_{\alpha} \underline{V_{\alpha}} h_{\alpha}$ is the transport of enthalpy by different species, and $\frac{p}{\rho} \sum_{\alpha=1}^{N_s} \frac{1}{Y_{\alpha}} \alpha_{\alpha}^T \underline{d}_{\alpha}$ is heat flux induced by pressure and/or body forces (also known as the Dufour effect). The thermal conductivity is evaluated via the Mason-Saxena formula [43],

$$\lambda = \sum_{\alpha=1}^{N_s} \lambda_{\alpha} \left[1 + \sum_{\beta \neq \alpha}^{N_s} G_{\alpha\beta} \frac{X_{\beta}}{X_{\alpha}} \right] \quad \text{with} \quad G_{\alpha\beta} = \frac{2}{5} L_{\alpha\beta}^* \frac{T}{p} \frac{\lambda_{\alpha}}{\alpha_{\alpha\beta}}, \tag{2.619}$$

where $L^*_{\alpha\beta}$ is a non-dimensional function involving the molecular weights of α and β and depends on exactly how the approximation is made. Thus, several contributions to transport include:

- Soret Effect: Diffusion of species due to a temperature gradient. Note that this effect tends to push light molecules such as hydrogen to hotter regions and heavy molecules such as soot and nitrogen to colder regions. This effect is also known as thermophoresis in the context of particulates [38, 6].
- Dufour Effect: Diffusion of heat/energy due to a concentration gradient [38].
- Diffusion by pressure gradients
- In general, second-order diffusion processes such as the Soret and Dufour effects are much smaller in magnitude than Fickian diffusion. Important exceptions in the context of combustion include transport of hydrogen against temperature gradients, wherein thermal diffusion can compete with Fickian diffusion, and the transport of heavy particulates such as soot down temperature gradients. Indeed, it is thermophoresis that ensures that soot particles formed in a diffusion flame tend to remain within the reaction zone. The Dufour effect, on the other hand, is generally negligible in combustion environments.

Discussion Box 4 : Physics and Conventions of Thermodiffusion

Thermophoresis, or the Soret effect, is generally observed at scales less than 1 mm. As small particles near a hot area are heated, they acquire greater kinetic energy and begin to push larger, slower-moving particles away from the heat source. The result of this phenomenon, which is generally referred to as thermodiffusion, is labeled positive when particles move from a hot to a cold region – thus, in general, heavier species exhibit positive thermodiffusive behavior while lighter species exhibit negative thermodiffusive behavior [16]. In addition to its important impact on several combustion systems such as those including high-hydrogen fuels, thermophoresis is critical in processes such as manipulating single biological molecules and adjusting impurity concentrations in semiconductor wafers.

2.6.4. Recap and Summary of Working Equations.

We can now summarize our presentation of the conservation equations,

Mass:
$$\partial_t \rho + \nabla \cdot (\rho \underline{u}) = 0$$
 (2.51)

Momentum:
$$\partial_t(\rho \underline{u}) + \nabla \cdot (\rho \underline{u} \otimes \underline{u}) = -\nabla p + \nabla \cdot \underline{\underline{\sigma}} + \sum_{\alpha=1}^{N_s} \rho Y_{\alpha} \underline{g_{\alpha}}$$
 (2.55)

Species:
$$\partial_t(\rho Y_\alpha) + \nabla \cdot (\rho \underline{u} Y_\alpha) = -\nabla \cdot \underline{j_\alpha} + \rho \dot{\omega}_\alpha$$
 (2.56)

Total Enthalpy:
$$\partial_t(\rho h_t) + \nabla \cdot (\rho \underline{u} h_t) = \partial_t p - \nabla \cdot q + \nabla \cdot (\underline{\sigma} \cdot \underline{u}) + \rho \sum_{\alpha=1}^{N_s} Y_\alpha \underline{g}_\alpha \cdot (\underline{u} + \underline{V}_\alpha)$$

$$(2.511)$$

State Relation:
$$p = \rho RT$$
 (2.11)

with the following constitutive relations,

$$\underline{\sigma} = \mu [\nabla \underline{u} + (\nabla \underline{u})^T] + (\kappa - 2\mu/3) \nabla \cdot \underline{u} \underline{I}$$
(2.62)

$$\mu = f(\underline{X}, T), \kappa$$
: bulk viscosity

$$\underline{j_{\alpha}} = -\rho \underline{V_{\alpha}} Y_{\alpha} \tag{2.57}$$

$$q = -\lambda \nabla T \tag{2.620}$$

2.7. Reaction Chemistry

Let us first consider the generic reaction sequence,

$$\sum_{\alpha=1}^{N_s} \nu'_{\alpha l} \mathbf{A}_{\alpha} \stackrel{k_f}{\underset{k_b}{\rightleftharpoons}} \sum_{\alpha=1}^{N_s} \nu''_{\alpha l} \mathbf{A}_{\alpha}, \quad l = 1, \dots, N_r$$
(2.71)

with N_r the number of reactions, A_{α} defining species α , and $\nu'_{\alpha l}, \nu''_{\alpha l}$ the molar coefficient of species α in reaction l. Note that we can also define \dot{m}_{α} as the chemical source term of species α in terms of w_l , the reaction rate for reaction l,

2.8. USEFUL SIMPLIFICATIONS

$$\dot{m}_{\alpha} = \rho \dot{\omega}_{\alpha} = W_{\alpha} \sum_{l=1}^{N_r} \nu_{\alpha l} w_l.$$
(2.72)

Further, we can write w_l as follows,

$$w_{l} = k_{f}^{l} \prod_{\alpha=1}^{N_{s}} [A_{\alpha}]^{\nu_{\alpha l}^{\prime}} - k_{b}^{l} \prod_{\alpha=1}^{N_{s}} [A_{\alpha}]^{\nu_{\alpha l}^{\prime\prime}}, \qquad (2.73)$$

where
$$[A_{\alpha}] = \frac{\rho Y_{\alpha}}{W_{\alpha}},$$
 (2.74)

in terms of k_f^l and k_b^l , the forward and backward rate coefficients of reaction l. These rate constants can be written in Arrhenius form,

$$k_f^l = A_l T^{\beta_l} \exp\left\{-\frac{E_{A,l}}{\mathcal{R}T}\right\},\tag{2.75}$$

and the backward rate constant is obtained from the equilibrium constant,

$$K = \frac{k_f}{k_b}.$$
(2.76)

2.8. Useful Simplifications

A number of useful assumptions can be invoked in order to simplify this analytic treatment, isolate individual combustion-physical processes, and reduce computational complexity. Common assumptions include:

- Isothermal combustion: useful for idealized DNS, analytical studies, and asymptotic investigations
 - $-~\rho=$ constant; enables consideration of Reynolds-averaging; neglect of dilatational effects
 - Constant transport properties
 - Reaction is passive and has no feedback on the hydrodynamic flowfield; used for instability theory
 - Transition analysis
- One-step chemistry: $\nu F + O \rightarrow (1 + \nu)P$, simplifies analysis by reducing chemical complexity
- Calorically perfect gas: $c_p = \text{constant}$, simplifies transport
- Equal, but temperature-dependent heat capacity (thermally perfect): $c_{p,\alpha} = c_p = f(T)$

• Equal species and thermal transport (i.e. diffusion):

$$\alpha_T = \alpha_\alpha \to Le_\alpha = \frac{\lambda}{\rho c_p \alpha_\alpha} = \frac{\alpha_T}{\alpha_\alpha} = 1$$
(2.81)

 \bullet Constant pressure (isobaric): p= constant; good approximation for low-Mach number deflagrations and diffusion flames ; Not valid for high-speed combustion or detonation

CHAPTER 3

Mathematical Analysis of Simple Flames

We will now proceed to apply the equations and formulation presented above to a coaxial jet flame. We will use this setting to review key equations and simplifications while also introducing important non-dimensionalizations.

3.1. Non-dimensionalization

To obtain a fundamental understanding of physical processes via mathematical models, it is convenient to non-dimensionalize the modeling equations. Non-dimensionalization tends to reveal the significance of related processes and timescales, identify the importance of individual terms in the overall solution, and enable self-similarity analysis. The process of non-dimensionalization often entails introducing appropriate reference quantities. To illustrate this, we consider a simple canonical problem of a jet diffusion flame [48]. In this situation, the combustion chemistry can be modeled by a global one-step reaction:



 $\nu_{\rm F}' \mathbf{F} + \nu_{\rm O}' \mathbf{O} \stackrel{k_f}{\rightharpoonup} \nu_{\rm P}'' \mathbf{P}. \tag{3.11}$

FIGURE 3.11 Diagram of a jet diffusion flame with diameter D_0 .

We can define reference quantities with respect to bulk properties and quantities of the jet such as the jet nozzle diameter D_0 , the bulk jet exit velocity u_0 , and properties of the

jet fluid such as viscosity ν_0 , thermal diffusivity α_0^T , heat capacity c_{pJ} , and density ρ_0 . To simplify our analysis, we can introduce the following simplifying assumptions:

- Low-speed combustion: compressibility effects are negligible and convective scaling is employed
- Equal species diffusivity: $\alpha_{\alpha} = \alpha$; unity Lewis number approximation
- Fick's law (via equal species diffusivity): $Y_{\alpha} \underline{V_{\alpha}} = -\alpha \nabla Y_{\alpha}$ see [50] for more details
- Constant and equal heat capacity: $c_{p,\alpha} = c_p$; calorically perfect gas
- Ideal gas: Eq. (2.11) applies
- Pressure decomposition: in low Mach number flows, we can decompose the pressure, we can introduce the Mach number M = u/c (with c the speed of sound) as the relevant parameter for an acoustic scaling. We can then expand the pressure using perturbation analysis as,

$$p = p_0 + M_0^2 p_2 + O(M_0^3), (3.12)$$

where p_0 is the thermodynamic pressure, which affects the equation of state, and p_2 is the hydrodynamic pressure, which affects the momentum equation.

With these assumptions, we can utilize the formulation of Sec. 2.5 to model the system,

Mass:
$$\partial_t \rho + \nabla \cdot (\rho \underline{u}) = 0$$
 (3.13a)

Momentum: $\partial_t(\rho \underline{u}) + \nabla \cdot (\rho \underline{u} \otimes \underline{u}) = -\nabla p_2 + \nabla \cdot \underline{\sigma} + \rho g$ (3.13b)

Fuel:
$$\partial_t(\rho Y_{\rm F}) + \nabla \cdot (\rho \underline{u} Y_{\rm F}) = -\nabla \cdot (\rho \alpha \nabla Y_{\rm F}) + W_{\rm F} \nu_{\rm F} w$$
 (3.13c)

Oxidizer:
$$\partial_t(\rho Y_{\rm O}) + \nabla \cdot (\rho \underline{u} Y_{\rm O}) = -\nabla \cdot (\rho \alpha \nabla Y_{\rm O}) + W_{\rm O} \nu_{\rm O} w$$
 (3.13d)

where,
$$w = A \exp\left\{-\frac{E_A}{\mathcal{R}T}\right\} \left(\frac{\rho Y_{\rm F}}{W_{\rm F}}\right)^{\nu_{\rm F}'} \left(\frac{\rho Y_{\rm O}}{W_{\rm O}}\right)^{\nu_{\rm O}'}$$
, (3.13e)

Energy:
$$\partial_t(\rho T) + \nabla \cdot (\rho \underline{u}T) = \nabla \cdot \left(\frac{\lambda}{c_p}\nabla T\right) + \frac{1}{c_p}\underline{\sigma} : \nabla \underline{u} + \underline{\dot{q}_T} + \frac{1}{c_p}(\partial_t p_0 + \underline{u} \cdot \nabla p_0),$$
(3.13f)

$$\underline{\dot{q}_T} = -\frac{1}{c_p} \sum_{\alpha=1}^{N_s} h_\alpha W_\alpha \nu_\alpha w, \qquad (3.13g)$$

where h_{α} combines the chemical and sensible enthalpies of species α . We now introduce the following nondimensional quantities:

$$\begin{aligned} x^{\dagger} &= \frac{x}{D_0}; \quad t^{\dagger} = \frac{tu_0}{D_0}; \quad u^{\dagger} = \frac{u}{u_0}; \quad p^{\dagger} = \frac{p}{\rho_0 u_0^2}; \quad \rho^{\dagger} = \frac{\rho}{\rho_0}; \quad \alpha^{\dagger} = \frac{\alpha}{\alpha_0} \\ \nu^{\dagger} &= \frac{\nu}{\nu_0}; \quad W_{\alpha}^{\dagger} = \frac{W_{\alpha}}{W}; \quad \underline{\sigma}^{\dagger} = \frac{D_0}{\rho_0 \nu_0 u_0} \underline{\sigma}; \quad T^{\dagger} = \frac{T}{T_b - T_u} = \frac{T}{\Delta T}; \quad h^{\dagger} = \frac{h}{c_{pJ} T_B} \end{aligned}$$

3.1. NON-DIMENSIONALIZATION

$$\begin{array}{ll} \partial_t{}^{\dagger} = \frac{D_0}{u_0}\partial_t; & \nabla^{\dagger} = D_0\nabla; & Y_{\alpha}{}^{\dagger} = \frac{Y_{\alpha}}{Y_0}; & Y_0 = 1; & \underline{\hat{e}}_g: \text{gravitational direction}; \\ Ze = \frac{E_A}{\mathcal{R}T_b}; & Ce = \frac{T_b - T_u}{T_b}; & T_A = \frac{E_A}{\mathcal{R}} \end{array}$$

With these definitions, we can rewrite the exponent in Arrhenius form as,

$$\frac{E_A}{\mathcal{R}T} = \frac{T_a}{T_b} \frac{T_b}{T} \tag{3.14}$$

$$= Ze\left(\frac{1}{CeT^{\dagger}}\right) \tag{3.15}$$

$$= Ze\left(\frac{1-CeT^{\dagger}}{CeT^{\dagger}}+1\right)$$
(3.16)

$$= Ze + \frac{Ze}{Ce} \left(\frac{1 - CeT^{\dagger}}{T^{\dagger}} \right)$$
(3.17)

$$\therefore \exp\left\{-\frac{E_A}{\mathcal{R}T}\right\} = \exp\{-Ze\} \exp\left\{-\frac{Ze}{Ce}\left(\frac{1-CeT^{\dagger}}{T^{\dagger}}\right)\right\}, \qquad (3.18)$$

With this expression, we can rewrite the non-dimensional chemical source term as,

$$w^{\dagger} = \frac{wW\nu_0}{u_0/D_0\rho_0},$$
(3.19)

where ν_0 is a reference net stoichiometric coefficient and W is a reference molecular weight. Similarly, the non-dimensional conservation equations become,

$$\text{Mass}: \partial_t^{\dagger} \rho^{\dagger} + \nabla^{\dagger} \cdot (\rho^{\dagger} \underline{u}^{\dagger}) = 0 \tag{3.110}$$

Momentum :
$$\partial_t^{\dagger}(\rho^{\dagger}\underline{u}^{\dagger}) + \nabla^{\dagger} \cdot (\rho^{\dagger}\underline{u}^{\dagger} \otimes \underline{u}^{\dagger}) = -\nabla^{\dagger}p^{\dagger} + \frac{1}{Re}\nabla^{\dagger} \cdot \underline{\underline{\sigma}}^{\dagger} + \frac{1}{Fr}\rho^{\dagger}\underline{\hat{e}}_{g}$$
 (3.111)

Energy:
$$\partial_t^{\dagger}(\rho^{\dagger}T^{\dagger}) + \nabla^{\dagger} \cdot (\rho^{\dagger}\underline{u}^{\dagger}T^{\dagger}) = \frac{Le}{ReSc} \nabla^{\dagger} \cdot \left(\rho^{\dagger}\alpha_T^{\dagger}\nabla^{\dagger}T^{\dagger}\right) + \frac{Ec}{Re} \frac{1}{c_p^{\dagger}} \underbrace{\sigma^{\dagger}}_{p} : \nabla^{\dagger}\underline{u}^{\dagger}$$
(3.112)

$$+ Da \frac{1}{c_p^{\dagger}} \sum_{\alpha=1}^{N_s} h_{\alpha}^{\dagger} W_{\alpha}^{\dagger} \nu_{\alpha}^{\dagger} w_{\alpha}^{\dagger} + Ec \frac{1}{c_p^{\dagger}} (d_t^{\dagger} p^{\dagger} + \underline{u}^{\dagger} \cdot \nabla^{\dagger} p^{\dagger})$$

We can also introduce the Damköhler number,

$$Da = \frac{\tau_{Flow}}{\tau_{Chem}} = \frac{\text{Characteristic Flow Time Scale}}{\text{Chemical Time Scale}} = \frac{D_0}{u_0} \left(\frac{W_0}{\rho_0}\right) \nu_0 \left(\frac{\rho_0}{W_0}\right)^{\nu_0 + \nu_F} \exp\{-Ze\}.$$

such that the species conservation equations take the form:

$$\begin{aligned} \partial_t^{\dagger}(\rho^{\dagger}Y_{\mathcal{O}}{}^{\dagger}) + \nabla^{\dagger} \cdot (\rho^{\dagger}\underline{u}^{\dagger}Y_{\mathcal{O}}{}^{\dagger}) &= \frac{1}{ReSc} \nabla^{\dagger} \cdot (\rho^{\dagger}\alpha^{\dagger}\nabla^{\dagger}Y_{\mathcal{O}}{}^{\dagger}) + DaW_{\mathcal{O}}^{\dagger}\nu_{\mathcal{O}}^{\dagger}w^{\dagger} \qquad (3.113a)\\ \partial_t^{\dagger}(\rho^{\dagger}Y_{\mathcal{F}}{}^{\dagger}) + \nabla^{\dagger} \cdot (\rho^{\dagger}\underline{u}^{\dagger}Y_{\mathcal{F}}{}^{\dagger}) &= \frac{1}{ReSc} \nabla^{\dagger} \cdot (\rho^{\dagger}\alpha^{\dagger}\nabla^{\dagger}Y_{\mathcal{F}}{}^{\dagger}) + DaW_{\mathcal{F}}^{\dagger}\nu_{\mathcal{F}}^{\dagger}w^{\dagger} \\ \text{with, } w^{\dagger} &= \exp\left\{-\frac{Ze}{Ce}\left(\frac{1-CeT^{\dagger}}{T^{\dagger}}\right)\right\} \left[\frac{\rho^{\dagger}Y_{\mathcal{F}}{}^{\dagger}}{W_{\mathcal{F}}{}^{\dagger}}\right]^{\nu_{\mathcal{F}}} \left[\frac{\rho^{\dagger}Y_{\mathcal{O}}{}^{\dagger}}{W_{\mathcal{O}}{}^{\dagger}}\right]^{\nu_{\mathcal{O}}}. \quad (3.113b)\end{aligned}$$

3.2. Non-dimensional Parameters

The non-dimensionalization procedure developed in Sec. 3.1 yields several key parameters that are important in understanding the relative effects of different physical phenomena:

$$\begin{array}{l} \mbox{Reynolds Number: } Re = \frac{u_0 D_0}{\nu_0} = \frac{\mbox{Inertial Forces}}{\mbox{Viscous Forces}} \\ \mbox{Schmidt Number: } Sc = \frac{\nu_0^\dagger}{\alpha_0^\dagger} = \frac{\mbox{Viscous Forces}}{\mbox{Diffusive Forces}} \\ \mbox{Lewis Number: } Le = \frac{\lambda_0}{c_{pJ}\rho_0\alpha_0} = \frac{\mbox{Thermal Diffusion}}{\mbox{Species Diffusion}} \\ \mbox{Damköhler Number: } Da = \frac{\tau_{Flow}}{\tau_{Chem}} = \frac{\mbox{Convective Time}}{\mbox{Chemical Time}} \\ \mbox{Zeldovich Number: } Ze = \frac{T_a}{T_b} = \frac{E_A}{\mathcal{R}T_b} = \frac{\mbox{Activation Temperature}}{\mbox{Fame Temperature}} \\ \mbox{Heat Release Parameter: } Ce = \frac{T_b - T_u}{T_b} = \frac{\mbox{Temperature Increase}}{\mbox{Fame Temperature}} \\ \mbox{Froude Number: } Fr = \frac{u_0^2}{gD_0} = \frac{\mbox{Inertial Force}}{\mbox{Gravitational Force}} \\ \mbox{Richardson Number: } Ri = \frac{1}{F_r} = \frac{gD_0}{u_0^2} = \frac{\mbox{Gravitational Force}}{\mbox{Inertial Force}} \\ \mbox{Eckhart Number: } Ec = \frac{u_0^2}{c_p\Delta T} = \frac{\mbox{Kinetic Energy}}{\mbox{Sensible Enthalpy}} \end{array}$$

Comparing terms obtained from convective and acoustic analysis, we find that for low-Mach flows, we can write the momentum equation as,

$$\partial_t^{\dagger}(\rho^{\dagger}\underline{u}^{\dagger}) + \nabla^{\dagger} \cdot (\rho^{\dagger}\underline{u}^{\dagger} \otimes \underline{u}^{\dagger}) = -\nabla^{\dagger}p_2^{\dagger} + \frac{1}{Re}\nabla^{\dagger} \cdot \underline{\underline{\sigma}}^{\dagger} + \frac{1}{Fr}\rho^{\dagger}\underline{\hat{e}_g}, \qquad (3.21)$$

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where the $\nabla^\dagger p^\dagger$ term is the hydrodynamic pressure. The non-dimensional form of the species equations becomes,

$$\partial_t^{\dagger}(\rho^{\dagger}Y_{\alpha}{}^{\dagger}) + \nabla^{\dagger} \cdot (\rho^{\dagger}\underline{u}^{\dagger}Y_{\alpha}{}^{\dagger}) = \frac{1}{ReSc} \nabla^{\dagger} \cdot (\rho^{\dagger}\alpha^{\dagger}\nabla^{\dagger}Y_{\alpha}{}^{\dagger}) + DaW_{\alpha}^{\dagger}\nu_{\alpha}^{\dagger}w^{\dagger}, \qquad (3.22)$$

and the temperature equation can be expressed as,

$$\partial_t^{\dagger}(\rho^{\dagger}T^{\dagger}) + \nabla^{\dagger} \cdot (\rho^{\dagger}\underline{u}^{\dagger}T^{\dagger}) = \frac{Le}{ReSc} \nabla^{\dagger} \cdot \left(\rho^{\dagger}\alpha_T^{\dagger}\nabla^{\dagger}T^{\dagger}\right) + \frac{Ec}{Re} \frac{1}{c_p^{\dagger}} \underbrace{\underline{\sigma}}_{p}^{\dagger} : \nabla^{\dagger}\underline{u}^{\dagger} + \qquad (3.23)$$
$$Da \frac{1}{c_p^{\dagger}} \sum_{\alpha=1}^{N_s} h_{\alpha}^{\dagger} W_{\alpha}^{\dagger} \nu_{\alpha}^{\dagger} w_{\alpha}^{\dagger} + \frac{\gamma - 1}{\gamma} \frac{T_0}{T_b} \frac{1}{Ce} \frac{1}{c_p^{\dagger}} (\partial_t^{\dagger}p^{\dagger} + \underline{u}^{\dagger} \cdot \nabla^{\dagger}p^{\dagger}),$$

where the term $\frac{\gamma-1}{\gamma} \frac{T_0}{T_b} \frac{1}{Ce}$ is O(1) and we used the relation,

$$\frac{c_0^2}{\gamma c_{pJ}\Delta T} = \frac{c_0^2}{\gamma \left(\frac{\gamma}{\gamma - 1}R_0T_0\right)} \frac{T_0}{T_b} \frac{T_b}{\Delta T},\tag{3.24}$$

with $T_0 = T_u$ the unburned gas temperature.

3.2.1. Reminders on Compressibility and Low-Mach Number Formulation. The non-dimensionalization presented in Sec. 3.2 allows us to identify key terms that can be neglected, simplifying analysis in various contexts. From convective scaling analysis, we found that the non-dimensional quantities Fr, Re, Sc, Da, and Ec become relevant parameters. Based on their magnitude and relative scaling, we can neglect their contribution. Alternatively, we could introduce an acoustic/compressible scaling by which we scale pressure by a reference pressure such that

$$p^{\dagger} = \frac{p}{p_0},\tag{3.25}$$

where p_0 is the characteristic pressure and u_0 is a characteristic velocity scale. Recognizing that $p_0 = \rho_0 c_0^2 / \gamma$ and that the jet exit Mach number is $M_0 = u_0 / c_0$, we can write the non-dimensional form of the momentum equation as,

$$\partial_t^{\dagger}(\rho^{\dagger}\underline{u}^{\dagger}) + \nabla^{\dagger} \cdot (\rho^{\dagger}\underline{u}^{\dagger} \otimes \underline{u}^{\dagger}) = -\frac{1}{\gamma} \frac{1}{M_0^2} \nabla^{\dagger} p^{\dagger} + \frac{1}{Re} \nabla^{\dagger} \cdot \underline{\underline{\sigma}}^{\dagger} + \frac{1}{Fr} \rho^{\dagger} \underline{\underline{\hat{e}}}_{g}.$$
(3.26)
Thus, in the limit of a low-Mach number flow, we can write the governing equations in the following (dimensional) form using the low Mach number pressure expansion of Eq. (3.12),

$$\partial_t \rho + \nabla \cdot \left(\rho \underline{u}\right) = 0 \tag{3.27a}$$

$$\partial_t(\rho \underline{u}) + \nabla \cdot (\rho \underline{u} \otimes \underline{u}) = -\nabla p_2 + \nabla \underline{\underline{\sigma}} + \rho g \hat{\underline{e}}_g$$
(3.27b)

$$\partial_t(\rho Y_\alpha) + \nabla \cdot (\rho \underline{u} Y_\alpha) = \nabla \cdot (\rho \alpha \nabla Y_\alpha) + W_\alpha \nu_\alpha w \tag{3.27c}$$

$$\partial_t(\rho T) + \nabla \cdot (\rho \underline{u}T) = \nabla \cdot (\rho \alpha_T \Delta T) + \frac{1}{c_p} \sum_{\alpha=1}^{N_s} h_\alpha W_\alpha \nu_\alpha w + \frac{1}{c_p} (\partial_t p_0 + \underline{u} \cdot \nabla p_0), \quad (3.27d)$$

along with the equation of state $p_0 = \rho RT$. For incompressible flows, we therefore decouple hydrodynamic and acoustic pressure, so that the density is independent of pressure perturbations. This can be illustrated by expanding the density around the thermodynamic pressure,

$$\rho(p_0 + \delta p, s, \underline{Y}) \approx \rho(p_0, s, \underline{Y}) + \left(\frac{\partial \rho}{\partial p}\right)_{s, \underline{Y}} \delta p, \qquad (3.28)$$

with $(\partial \rho / \partial p|_s = 0)$. Recognizing that $c^2 = (\partial p / \partial \rho|_{s,\underline{Y}})$, we find that the pressure perturbation will propagate with infinite sound speed such that $c \to \infty$ in the low-Mach limit.

3.3. Mixture-Fraction and Coupling Function

Here we extend our discussion of mixture fraction that we introduce in Sec. 2.3. For diffusion flames it is convenient to characterize the local mixing, which is a conserved scalar (but not a passive one). There are several main advantages to this approach. First, the conserved scalar provides a convenient representation of the local mixing. Secondly, it enables the representation of reaction chemistry in terms of a reduced set of scalars – that is, $(\underline{Y}, T, w, ...) = f(Z)$. A specific example would be the Burke-Schumann solution (the thin flame sheet approximation).

The mixture fraction can be introduced by first defining a coupling function(a nonnormalized mixture fraction), which is most easily accomplished if we consider the one-step chemistry,

$$\nu'_{\rm F} F + \nu'_{\rm O} O \to \nu''_{\rm P} P \tag{3.31}$$

with unity Lewis number, meaning that thermal and species are characterized by equal diffusivities. We can now define a general transport operator \mathcal{L} such that,

$$\mathcal{L}(Y) = \rho \partial_t Y + \rho \underline{u} \cdot \nabla Y - \nabla \cdot (\rho \alpha \nabla Y), \qquad (3.32)$$

which allows us to write the species transport equations as,

$$\mathcal{L}(Y_{\rm F}) = W_{\rm F} \nu_{\rm F} w, \qquad (3.33)$$

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$$\mathcal{L}(Y_{\rm O}) = W_{\rm O}\nu_{\rm O}w. \tag{3.34}$$

Linearly combining these equations allows us to eliminate the right-hand side, leaving us with,

$$\frac{W_{\rm O}\nu_{\rm O}}{W_{\rm F}\nu_{\rm F}}\mathcal{L}(Y_{\rm F}) - \mathcal{L}(Y_{\rm O}) = 0$$
(3.35)

Since the operator is linear, we can write the coupling function as,

$$\xi = \nu Y_{\rm F} - Y_{\rm O},\tag{3.36}$$

where ν is defined as in Eq. (2.24). From this, a normalized coupling function describing the mixture fraction is derived:

$$Z = \frac{\xi - \xi_{\rm O}}{\xi_{\rm F} - \xi_{\rm O}},\tag{3.37}$$

By relating density, species, temperatures, and other quantities to the mixture fraction, we can reduce our problem to solving the following equations:

$$\rho D_t \underline{u} = -\nabla p + \nabla \cdot \underline{\sigma} + \rho g \tag{3.38}$$

$$\rho D_t Z = \nabla \cdot (\rho \alpha \nabla Z) \tag{3.39}$$

where the last expression is obtained from the Burke-Schumann solution. This definition of the mixture fraction is strictly valid only for one-step chemistry. The important question then becomes: how can we derive a mixture fraction for a general problem that contains both preferential diffusion and multiple species? Fortunately, a more general definition can be obtained by recognizing conservation of elements. We first define the elemental mass fraction of element β (e.g. C, O, H, etc.) as,

$$y_{\beta} = \sum_{\alpha=1}^{N_s} \frac{n_{\alpha,\beta} W_{\beta}}{W_{\alpha}} Y_{\alpha}, \qquad (3.310)$$

with $n_{\alpha,\beta}$ the number of atoms of element β in species α , W_{β} the molecular weight of element β , W_{α} the molecular weight of species α , and Y_{α} the mass fraction of species α . As an example, we can compute $y_{\rm C}$ and $y_{\rm O}$ for a CO-CO₂-O₂ mixture as,

$$y_{\rm C} = \frac{W_{\rm C}}{W_{\rm CO}Y_{\rm CO}} + \frac{W_{\rm C}}{W_{\rm CO_2}}Y_{\rm CO_2}$$
(3.311)

$$y_{\rm O} = \frac{W_{\rm O}}{W_{\rm CO}} Y_{\rm CO} + \frac{2W_{\rm O}}{W_{\rm CO_2}} Y_{\rm CO_2} + \frac{2W_{\rm O}}{W_{\rm O_2}} Y_{\rm O_2}.$$
(3.312)

By introducing,

$$y = \zeta_{\rm C} y_{\rm C} + \zeta_{\rm O} y_{\rm O} + \zeta_{\rm H} y_{\rm H}, \qquad (3.313)$$

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with the weights ζ_i added to get compositional balance, we obtain,

$$Z = \frac{y - y_{\rm O}}{y_{\rm F} - y_{\rm O}}; \quad y = \frac{2}{W_{\rm C}}y_{\rm C} + \frac{1}{2W_{\rm H}}y_{\rm H} - \frac{1}{W_{\rm O}}y_{\rm O}$$
(3.314)

As a final remark, it is important to remember that for spray flames, we can identify a mixture fraction that is associated with the gaseous and liquid phases, as detailed in Discussion Box 2.

Discussion Box 5: Reduced Mechanisms for Methane-Air Combustion

While we have performed our analysis here considering a one-step global reaction, in reality, a great deal of academic work has been devoted to determining reaction pathways (or mechanisms) that can be used to compute the chemical source terms in both the species conservation and energy equations. Key considerations in forming these reaction mechanisms include agreement with experiment on key parameters (e.g. species and temperature profiles) and computational cost. The work of [4], for instance, demonstrates the reduction of a detailed 58-species mechanism for methane-air combustion to a four-species reduced mechanism, which reproduces behavior of the detailed mechanism to a degree that is useful in simulations wherein it is helpful to minimize computational cost of the chemical source terms. This issue is discussed in further detail in Sec. 5.2.

3.4. Self-Similarity and Structure of Laminar Flames

In preparation for transition and turbulent flame analysis, it is convenient to revisit the similarity structures of flames. For this analysis, we consider a jet diffusion flame and utilize the mixture fraction concept. A similar presentation can be found in [38], and a diagram of the system can be found in Fig. 3.41



FIGURE 3.41 Coordinate system for the self-similar jet diffusion flame.

3.4. SELF-SIMILARITY AND STRUCTURE OF LAMINAR FLAMES

We begin with the governing equations developed previously,

$$D_t \rho = -\rho \nabla \cdot \underline{u} \tag{3.41a}$$

$$\rho D_t u = -\nabla p + \nabla \cdot \underline{\sigma},\tag{3.41b}$$

$$\rho D_t Z = \nabla \cdot (\rho \alpha \nabla Z), \qquad (3.41c)$$

$$(\rho, \nu, \alpha) = f(Z), \tag{3.41d}$$

where the last expression means that all thermodynamics information depends explicitly on the mixture fraction. The following key assumptions are important:

- Equal and constant viscous-diffusive properties $(\alpha_{\alpha} = \alpha \rightarrow Sc = 1)$
- No gravitational effects: $Fr \to \infty$
- Steady-state
- Surrounding air is at rest
- ν constant
- Pressure in the flow is uniform
- Neglect mass diffusion and viscous effects in the axial direction

Using the non-dimensionalization introduced in Sec. 3.1, the steady-state governing equations in non-dimensional polar form become,

$$\frac{\partial}{\partial x}(\rho u) + \frac{1}{r}\frac{\partial}{\partial r}(\rho vr) = 0, \qquad (3.42)$$

$$\frac{\partial}{\partial x}(\rho u u) + \frac{1}{r}\frac{\partial}{\partial r}(\rho u v r) = \frac{1}{Re}\frac{1}{r}\frac{\partial}{\partial r}\left(\rho r\frac{\partial u}{\partial r}\right),\tag{3.43}$$

$$\frac{\partial}{\partial x}(\rho u Z) + \frac{1}{r}\frac{\partial}{\partial r}(\rho Z r) = \frac{1}{ReSc}\frac{1}{r}\frac{\partial}{\partial r}\left(\rho r\frac{\partial Z}{\partial r}\right).$$
(3.44)

Note that Eq. (3.42) is not technically needed because pressure is assumed to be constant. Appropriate boundary conditions can be stated as,

$$r = 0: \quad \frac{\partial u}{\partial r} = 0; \quad v = 0; \quad \frac{\partial Z}{\partial r} = 0$$
 (3.45)

$$r \to \infty: \quad u = 0; \quad v = 0; \quad Z = 0 \tag{3.46}$$

We can now rewrite the governing equations as,

Continuity:
$$\frac{\partial}{\partial x}(\rho ur) + \frac{\partial}{\partial r}(\rho vr) = 0,$$
 (3.47)

Axial Momentum:
$$\rho ur \frac{\partial}{\partial x} u + \rho vr \frac{\partial}{\partial r} u = \frac{1}{Re} \frac{\partial}{\partial r} \left(\rho r \frac{\partial}{\partial r} u \right),$$
 (3.48)

Mixture Fraction:
$$\rho ur \frac{\partial}{\partial x} Z + \rho vr \frac{\partial}{\partial r} Z = \frac{1}{ReSc} \frac{\partial}{\partial r} \left(\rho r \frac{\partial}{\partial r} Z \right);$$
 (3.49)

We can also introduce the Howarth transformation, which will re-parameterize system variables in a manner that simplifies mathematical analysis. Using the definitions,

$$\xi = x, \tag{3.410}$$

$$\hat{r} = \left(2\int_{0}^{r} \rho r' dr'\right)^{1/2}, \qquad (3.411)$$

$$\eta = \frac{\hat{r}(r)}{\xi}, \qquad (3.412)$$

where η is the spreading ratio. Applying this transformation allows for deriving self-similar equations for axial velocity and mixture fraction that admit an analytic solution. Deriving this set of equations is left as homework.

Discussion Box 6: Instabilities in unsteady diffusion flames.

While the classical analysis presented here deals with a steady diffusion flame under a variety of simple assumptions, even this relatively simple configuration is commonly studied in combustion science. In the work of [55], for instance, an analysis is performed to understand the impact of various model parameters (thermodynamic properties, viscousdiffusive transport, reaction chemistry, etc.) on the development of flow instabilities in jet diffusion flames. Results indicate that, for instance, certain approximations for expressing the viscosity and diffusivity can numerically damp hydrodynamic instabilities. Further, use of a one-step global reaction mechanism as opposed to detailed chemistry can also significantly attenuate important instability modes. From a practical standpoint, such instabilities can be quite important in the design of practical nonpremixed systems, as they can enhance mixing in a way that can result in improved performance. Thus, it is critical to consider the effect of each modeling choice one makes in a turbulent combustion context, even in flows that might at first glance seem relatively simple.

CHAPTER 4

Transition and Turbulence

4.1. Scaling and Nondimensionalization

Turbulent flows require consideration of interaction between different spatio-temporal scales. Indeed, turbulence is controlled by inertial effects such as non-linear convective processes. The key relevant parameter in defining turbulence and its associated transition is the Reynolds number, Re, defined in Sec. 3.2. Let us now consider both non-reacting and reacting turbulent jets, as shown in Fig. 4.11. From turbulence theory and self-similarity analysis, we know that jet momentum is conserved in the high-Re limit by integration of Eq. (3.111) assuming constant pressure and $Fr \to \infty$,

$$\partial_x(\rho u_x u_x) = 0 \to \rho u_x^2 A(x) = \rho u_0^2 A_0.$$
(4.11)

Further, we can define a local jet Reynolds number as,

$$Re_{1/2} = \frac{u_x r_{1/2}}{\nu},\tag{4.12}$$

with $r_{1/2}$ the jet half width, u_x the centerline velocity, and ν the local kinematic viscosity. From the self-similarity analysis of Sec. 3.4, we know that,

$$u_x \sim \left(\frac{x}{D_0}\right)^{\alpha}; \quad r_{1/2} \sim \left(\frac{x}{D_0}\right)^{\beta}; \quad \alpha \sim \frac{1}{\beta}$$
 (4.13)

where for a non-reacting jet, the local Reynolds number remains constant (with ν constant). In the case of a reacting jet, the effects of temperature variation on viscosity through Eq. (2.63),

$$\nu \sim \nu_0 \left(\frac{T}{T_0}\right)^m,\tag{4.14}$$

where the value of m = 5/2 is from the Sutherland approximation. Excellent work on this subject was performed by [46].

Now, assuming similar scaling for the velocity and jet radius, we can observe that the reacting jet introduces a dependence of the local Reynolds number on temperature and the potential for relaminarization, as shown in Fig. 4.12,



FIGURE 4.11 Diagram of a turbulent jet.

$$u_x \sim \left(\frac{x}{D_0}\right)^{\alpha'}; \quad \left(r_{1/2} \sim \frac{x}{D_0}\right)^{\beta'}$$

$$(4.15)$$

$$Re_{1/2}^{R} = \frac{u_{x}r_{1/2}}{\nu_{0}} \left(\frac{T}{T_{0}}\right)^{m} = Re_{1/2} \left(\frac{T}{T_{0}}\right)^{m}$$
(4.16)



FIGURE 4.12 Differences in behavior of local jet Reynolds number for reacting and nonreacting turbulent jets.

4.2. Transition of Laminar Jet Flames

As shown in Fig. 4.21, a variety of different mechanisms contribute to the transition to turbulence – viscosity, heat release, and dilatation all play important roles. The effects of heat release in particular are detailed in Discussion Box 7.



FIGURE 4.21 Mechanisms for transition to turbulence.

Discussion Box 7: Effects of heat release on turbulent flows

The work of [41] investigated the effect of various aspects of heat release on key aspects of turbulent flows via a series of detailed LES calculations. Simulations for both isothermal and reactive jets showed good agreement with available experimental data for the centerline velocity and scalar decay, and also jet half widths. Further, the simulations showed that the quasilaminarization of the shear layer surrounding the jet core region is mainly induced by the increase in viscosity and diffusivity due to heat-release, rather than dilatation effects. Contributions of the fluctuating mass flux to the overall mass flux were also shown to be contribute as much as 15 % to the total mass flux. This last observation is particularly important, as this term is often neglected in experimental studies due its difficult measurement.

The transition of laminar jet flames in particular can be studied using classical linear stability theory [57]. In general, transition is controlled by two key quantities: a Kelvin-Helmholtz mode that dominates the inviscid shear layer and a buoyancy-driven instability mode. To study the instability mode, one can develop a set of temporal and spatial instability analyses by decomposing a solution vector as,

$$\phi = (\rho, \underline{u}, T, p)^T \tag{4.21}$$

with $\underline{u} = (u, v, w)$ and mean and fluctuating quantities,

$$\underline{\phi}(\underline{x},t) = \overline{\phi}(x) + \underline{\phi}'(\underline{x},t) \tag{4.22}$$

Neglecting viscous effects and heat-release, one can write,

$$\partial_t \rho' + \nabla \cdot (\overline{\rho} \underline{u}' + \rho' \underline{\overline{u}}) = 0 \tag{4.23a}$$

$$\partial_t(\bar{\rho}\underline{u}') + \partial_t(\rho'\underline{\overline{u}}) + \nabla \cdot (\rho'\underline{\overline{u}} \otimes \underline{\overline{u}} + \overline{\rho}\underline{\overline{u}} \otimes \underline{u}') = -\nabla p' + \nabla \cdot \underline{\underline{\sigma}}' + g\rho'\underline{\hat{e}_g}$$
(4.23b)

$$\partial_t(\overline{\rho}T') + \partial_t(\rho'\overline{T}) + \nabla \cdot (\rho'\underline{u}\overline{T} + \overline{\rho}\underline{u}'\overline{T} + \overline{\rho}\underline{u}T') =$$
(4.23c)

$$D_t p' - \nabla \cdot \underline{q}' + \underline{\underline{\sigma}}' : \nabla \underline{\overline{u}} + \underline{\overline{\underline{\sigma}}} : \nabla \underline{\underline{u}}' + \rho' \sum_{\alpha = 1}^{N_s} Y_\alpha \underline{g_\alpha} \cdot \underline{V_\alpha},$$

where a planar wave approximation can be used to represent any of the fluctuating quantities,

$$\phi' = \hat{\phi}(r) \exp\{-i(\omega t - m\theta - \alpha x)\},\tag{4.24}$$

in terms of a temporal fluctuation frequency ω , an axial wavenumber α , and an azimuthal mode number m. In this model instabilities are governed by linear growth rates, and the system represented by Eq. (4.23a) - Eq. (4.23c) is converted to a set of ODEs that can be solved using a shooting method. To investigate spatial instabilities, we would prescribe $\omega \in \mathbb{R}$ and solve for $\alpha \in \mathbb{C}$ to obtain a plot such as that shown in Sec. 4.2. To investigate temporal instabilities, we would do the reverse: prescribe $\alpha \in \mathbb{R}$ and solve for $\omega \in \mathbb{C}$.



FIGURE 4.22 Growth rate plot for spatial instability analysis.

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Discussion Box 8: Flickering instability in diffusion flames

Low frequency flame oscillations, also known as the flame flicker and flare, have been observed for some time. Interestingly, the flicker frequency observed in nonpremixed and partially premixed flames is relatively independent of key parameters such as fuel type, nozzle size, and jet exit velocity. While a variety of different hypotheses and conjectures were proposed to explain the phenomenon, Buckmaster and Peters [] eventually showed that a modified Kelvin-Helmholtz type instability exists in diffusion flames, predicting a low frequency oscillation around 17 Hz. The instability is due to a buoyancy-induced velocity field which surrounds a forced convective flow. It was further speculated that the vortical structures outside the luminous flame are due to buoyancy-driven instability and are also responsible for the low frequency flame oscillation.

As a followup to this work, a stunning planar visualization of the outer vortices was performed by [14]. The frequency of the vortical structure outside the luminous flame was found to correlate with the flame oscillation frequency, generally found to be in the range of 10 Hz - 20 Hz. This flame oscillation frequency showed a weak dependence on burner exit velocity and coflowing annulus air, and the frequency increased as the burner exit velocity or the coflowing air velocity was increased. Buoyancy-driven toroidal vortices were also shown to exert significant stretching on the flame surface, which can locally quench an otherwise continuous flame surface and result in a detached flame puff. Thus, it became clear that buoyancy driven vortices are important to the dynamics of the flame at low and transitional Reynolds number conditions, at the least. This is an excellent example of a study that used a combination of first-principles theory and experiment to understand key characteristics of important combustion systems.

4.3. Turbulence

4.3.1. Statistical Analysis. Turbulent flows involve a wide rage of spatio-temporal scales and random motion. To describe turbulence, we therefore follow the usual statistical approach wherein we consider a scalar flow field variable $\zeta(\underline{x}, t)$,

$$\zeta = \{\underline{u_i}, T, \underline{Y} \dots\}. \tag{4.31}$$

We can introduce a Reynolds-decomposition:

$$\phi = \overline{\phi} + \phi', \tag{4.32}$$

where $\overline{\phi}$ is an averaged field and ϕ' is a fluctuating field quantity. In general, both $\overline{\phi}$ and $\phi' = \zeta'$ are generally functions of both space and time. We can distinguish between statistically stationary, spatially homogeneous, and statistically periodic as in Fig. 4.31. Statistically stationary variables have a consistent integrated average in time, spatially homogeneous variables have a consistent integrated average in space, and statistically periodic variables are expected to take the same average value at time intervals of a specified period T.

A more general (and equal) representation for the mean quantity is obtained by introducing a statistical approach. For this, we consider a Probability Density Function (PDF) of ϕ , where \underline{x} and t denote spatio-temporal dependence,

$$P_{\zeta}(\underline{x},t). \tag{4.33}$$



FIGURE 4.31 Demonstrations of statistical stationarity

The cumulative distribution function can also be defined such that,

$$F(\zeta) = \int_{-\infty}^{\zeta} P(\zeta') d\zeta', \qquad (4.34)$$

where it immediately follows that $P(\phi) = dF(\phi)/d\phi$. This is illustrated graphically in Fig. 4.32.

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This PDF has several additional properties – note that we use ξ and ζ as below as scalar sample space variables:

- $P(\phi) > 0$ $\int_{-\infty}^{\infty} P(\phi) d\phi$
- $P(a \le \phi \le b) = \int_a^b P(\phi) d\phi$ Joint PDF: $P(\xi, \zeta)$
- Marginal PDF:

$$P(\xi) = \int P(\xi, \zeta) d\zeta \tag{4.35}$$

$$P(\zeta) = \int P(\xi, \zeta) d\xi \tag{4.36}$$

• From Bayes' theorem, we can derive a conditional PDF $P(\zeta|\xi) = \frac{P(\xi,\zeta)}{P(\xi)}$

Importantly, the moments of a distribution can be expressed in terms of traditional terminology as,

Mean :
$$E[\xi] = \langle \xi \rangle = \int \xi P(\xi) d\xi,$$
 (4.37)

Variance:
$$Var[\xi] = \langle \zeta^2 \rangle = \int (\xi - \langle \xi \rangle)^2 P(\xi) d\xi,$$
 (4.38)

nth Moment:
$$\langle \xi'^n \rangle = \int (\xi - \langle \xi \rangle)^n P(\xi) d\xi,$$
 (4.39)

with n = 3 defining the skewness ("degree of asymmetry") and n = 4 the kurtosis ("peakedness").

Later, we will consider a mixture-fraction model for non-premixed flames and conditional moment closures (CMC). This model relies on conditional PDFs such as P(Y|Z), P(T|Z), and P(C|Z).

Furthermore, many combustion models such as flamelet models or models for premixed combustion utilize presumed PDF approaches to model the statistical distribution of scalar variables.

As an example of a joint PDF, we can consider a deterministic adiabatic flame temperature problem. Here, we can generalize this analysis to a case wherein we know the functional relation between two scalars. To illustrate the idea of joint, conditional, and marginal PDFs, let us assume that we have two random variables x and y such that,

$$x \in [-1,1]$$
 (4.310)

$$y \in [0,1] \tag{4.311}$$

$$y = 1 - x^2, (4.312)$$



FIGURE 4.32 Illustration of PDF and CDF

The joint PDF is then given as,

$$P(x,y) = \frac{1}{2}\delta(f),$$
(4.313)

with $f = y - 1 + x^2$, where δ is the delta function and the coefficient 1/2 is introduced such that,

$$\iint P(x,y)dxdy \equiv 1. \tag{4.314}$$

The marginal PDF for x can then be found as,

$$P(x) = \int_0^1 P(x, y) dy = \frac{1}{2} \left[\mathcal{H}(x+1) - \mathcal{H}(x-1) \right] = \begin{cases} 0 & x \le -1 \\ \frac{1}{2} & -1 \le x \le 1 \\ 0 & 1 \le x \end{cases}$$
(4.315)

where \mathcal{H} is the Heaviside function. Similarly,

$$P(y) = \int_{-1}^{1} P(x, y) dx = \frac{1}{2} \frac{1}{\sqrt{1 - y}}.$$
(4.316)

With this we can evaluate the conditional PDF as,

$$P(y|x) = \frac{P(x,y)}{P(x)} = \delta(y - 1 + x^2).$$
(4.317)

In graphical form, we can illustrate the different PDFs as shown in Fig. 4.33:



FIGURE 4.33 Illustration of conditional, marginal, and joint PDFs for $P(x,y)=\delta(y-1+x^2)$

Recall from distribution analysis:

$$\int \delta(y-a)dy = \mathcal{H}(y-a) = \begin{cases} 0 & y < a\\ 1 & y > a \end{cases},$$
(4.318)

with $a = (1 - x^2)$ we have for indefinite integration:

$$\int \delta[y - (1 - x^2)] dy = \mathcal{H}[y - (1 - x^2)].$$
(4.319)

By considering the bounds on y ($y \in [0,1]$), we can find constraints on x such that $y - (1 - x^2) = 0$ for $y \in [0,1]$. This condition is always fulfilled for,

$$y \ge (1 - x^2) - 1 \le x \le 1,$$
 (4.320)

with this we can rewrite,

$$\mathcal{H}[y - (1 - x^2)] = \mathcal{H}[y - (1 - x)(1 + x)]$$
(4.321)

$$= \frac{1}{2} [\mathcal{H}(1-x) + \mathcal{H}(1+x)], \qquad (4.322)$$

or, in functional form,

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$$P(x) = \begin{cases} 0 & x < 1\\ \frac{1}{2} & -1 \le x \le 1\\ 0 & x > 1 \end{cases}$$
(4.323)

4.3.1.1. Common Probability Density Functions. Examples of distributions that are commonly used for representation of turbulence-chemistry interaction in reacting flow situation can be characterized by knowledge of a few moments and the conditions under which turbulence-chemistry interaction occurs. These include the following:

• Dirac Distribution:

$$P(\phi) = \alpha \delta(\phi - \phi^{-}) + (1 - \alpha) \delta(\phi - \phi^{+}), \qquad (4.324)$$

For premixed combustion, $\phi \to T$, $\phi^- \to T_u$, $\phi^+ \to T_b$

• Gaussian PDF:

$$P(\phi) = \frac{1}{2\pi\sigma^2} \exp\left\{-\frac{(\phi - \overline{\phi})^2}{2\sigma^2}\right\},\tag{4.325}$$

with σ the standard deviation and $\overline{\phi}$ the mean value of ϕ . Some quantities that can take Gaussian PDFs include the velocity.

• Beta PDF:

$$P(\phi) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \phi^{a-1} \phi^{b-1}, \quad \phi \in [0,1],$$
(4.326)

with $a = \overline{\phi}\gamma$, $b = (1 - \overline{\phi})\gamma$, $\gamma = \frac{\overline{\phi}(1 - \overline{\phi})}{\overline{\phi'}^2} - 1$, and the gamma-function $\Gamma(\xi) = \int_0^\infty t^{\xi - 1} e^{-t} dt$. Note that for mixture fraction, $\zeta = Z$, and for the progress variable, $\xi = C$.

• Log-normal PDF:

$$P(\phi) = \frac{1}{\phi\sigma\sqrt{2\pi}} \exp\left\{-\frac{(\ln\phi - \mu)^2}{2\sigma^2}\right\}, \quad \phi > 0,$$
(4.327)

• Statistically Most Likely PDF:

Consider the functional S,

$$S(P(\phi)) = -\int_{-\infty}^{\infty} P(\phi) \ln\left(\frac{P(\phi)}{Q(\phi)}\right) d\phi, \qquad (4.328)$$

formally defined as the Kullback – Leibler divergence from distribution Q to distribution P. In this context, note that Q represents a priori PDF that can be used to bias the composition state. Minimizing S over all possible $P(\phi)$ provides

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an analytic expression for the so-called statistically most likely distribution that minimizes the entropy,

$$P_N(\phi) = Q(\phi) \exp\left\{\sum_{j=0}^N a_j \phi^j\right\},\tag{4.329}$$

where the N-dimensional parameter vector \underline{a} can be determined by constraining the Kullback-Leibler divergence. Conservation of moments can be generally expressed as,

$$\int P(\phi)_N d\phi = 1 \tag{4.330}$$

$$\int \phi P(\phi)_N d\phi = \overline{\phi} \tag{4.331}$$

$$\int (\phi - \overline{\phi})^j P_N(\phi) d\phi = \overline{\phi'^j}, \ j = 2...N.$$
(4.332)

Note that $S \to 0$ implies $\overline{\phi'^2} \to 0$, and conversely $S \to \infty$ implies $\overline{\phi'^2} \to \infty$.

4.3.2. Averaging Procedures.

4.3.2.1. *Reynolds Averaging.* For flows with *constant density* (isothermal systems), we commonly employ a Reynolds-averaging procedure:

$$\phi = \overline{\phi} + \phi' \to \overline{\overline{\phi}} \equiv \overline{\phi}; \quad \overline{\phi'} \equiv 0 \tag{4.333}$$

$$\rho\phi = (\overline{\phi} + \rho')(\overline{\phi} + \phi') \tag{4.334}$$

$$=\overline{\rho}\overline{\phi} + \overline{\rho}\phi' \text{ with } \rho' = 0, \quad \rho = \text{const}$$

$$(4.335)$$

$$\therefore \nabla \cdot (\overline{\rho}\underline{u}) = \nabla \cdot (\rho \overline{\underline{u}}) \tag{4.336}$$

4.3.2.2. *Favre Averaging.* However, the application of the Reynolds-averaging to variable density flows introduced additional unclosed terms that require modelling. This can be shown by:

$$\rho\phi = \overline{\rho}\phi + \overline{\rho}\phi' + \rho'\phi + \rho'\phi' \qquad (4.337)$$

$$\therefore \partial_t \overline{\rho} + \nabla \cdot (\overline{\rho \underline{u}}) = \partial_t \overline{\rho} + \nabla \cdot (\overline{\rho \underline{u}} + \overline{\rho' \underline{u}'}) = 0, \qquad (4.338)$$

in which the density-velocity correlation $\overline{\rho'\underline{u}'}$ appears as an unclosed term that requires modelling. To avoid density correlations, we therefore introduce the *Favre Averaging* (mass

averaging):

$$\phi = \widetilde{\phi} + \phi'' \tag{4.339}$$

Definition:
$$\overline{\rho\phi} = \rho\widetilde{\phi} \to \widetilde{\phi} = \frac{\rho\phi}{\overline{\rho}}; \quad \widetilde{\phi''} = 0.$$
 (4.340)

We can prove this last statement in the following way:

$$\widetilde{\phi''} = 0 \tag{4.341}$$

$$\therefore \widetilde{\phi''} = \frac{\rho(\phi - \widetilde{\phi})}{\overline{\rho}} = \frac{\overline{\rho\phi}}{\overline{\rho}} - \frac{\overline{\rho\phi}}{\overline{\rho}}, \qquad (4.342)$$

Thus, we can reach the important conclusion that,

$$\partial_t \overline{\rho} + \nabla \cdot (\overline{\rho \underline{u}}) \to \nabla \cdot (\overline{\rho} \underline{\widetilde{u}}) = 0. \tag{4.343}$$

Note that Favre-averaging can be performed in volumetric or temporal senses by extending the averaging procedures:

$$\widetilde{\phi} = \frac{1}{V} \frac{1}{\overline{\rho}} \iiint_{V} \rho \phi dV \tag{4.344}$$

$$\widetilde{\phi} = \frac{1}{T} \frac{1}{\overline{\rho}} \int_{t}^{t+T} \rho \phi dt \qquad (4.345)$$

$$\widetilde{\phi} = \frac{1}{\rho} \int \rho \phi P(\phi) d\phi.$$
(4.346)

4.3.3. Filtering. While Reynolds-Averaged-Navier-Stokes (RANS) methods and one-point closures typically consider a statistical approach, *Large-Eddy Simulation* (LES) introduces a time-resolved formulation in which the largest turbulent scales are resolved in space and time while only the effects of the smallest scales are modeled. LES can be considered as a low-pass filter of the instantaneous solution, where filtered quantities are obtained by applying the following procedure:

Reynolds Filter:
$$\begin{cases} \overline{\phi}(\underline{x},t) = \int_{-\infty}^{\infty} \phi(\underline{x}-\underline{x}',t) G(\underline{x}';\Delta) dx' \\ \phi'(\underline{x},t) \phi(\underline{x},t) - \overline{\phi}(\underline{x},t) \end{cases}$$
(4.347)
Favre Filter:
$$\begin{cases} \overline{\phi}(\underline{x},t) = \frac{1}{\overline{\rho}} \int_{-\infty}^{\infty} \rho(\underline{x}-\underline{x}',t) \phi(\underline{x}-\underline{x}',t) G(\underline{x}';\Delta) dx' \\ \phi''(\underline{x},t) \phi(\underline{x},t) - \widetilde{\phi}(\underline{x},t) \end{cases}$$
(4.348)

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More generally, by introducing a space-time filter, we can write,

$$\overline{\phi}(\underline{x},t) = \iint_{-\infty}^{+\infty} \phi(\underline{x}-\underline{x}',t-t')G(\underline{x}',t',\Delta_x,\Delta_t)d\underline{x}'dt.$$
(4.349)

Typical filter operators include the following – it is often advantageous to convert to a Fourier representation to understand the spectral properties of these filters – Fig. 4.34 explicitly illustrates the profile of these functions in spectral space.

• Top-Hat Filter:

$$\begin{cases} G(x - x') = \frac{1}{\Delta} \text{ if } (x - x') \le \Delta/L \\ \widehat{G}(\kappa) = \operatorname{sinc}(\kappa \Delta/2) \end{cases}$$
(4.350)

• Gaussian Filter:

$$\begin{cases} G(x - x') = \frac{\xi}{\pi \Delta^2} \exp\{-\frac{\xi(x - x')^2}{\Delta^2}\} \\ \widehat{G}(\kappa) = \exp\{-\frac{(\Delta \kappa)^2}{4\xi}\} \end{cases}$$
(4.351)

• Sharp Spectral Cut-off:

$$\begin{cases} G(x-x') = \frac{\sin(\kappa_C(x-x'))}{\kappa_C(x-x')}; & \kappa_C = \frac{\pi}{4} \\ \widehat{G}(\kappa) = \begin{cases} 1 \text{ if } \kappa < \kappa_C \\ 0 \text{ else} \end{cases}$$
(4.352)

4.3.4. Correlations, Energy Spectrum, and Turbulent Scales. Turbulence is characterized by coherent spatio-temporal scales. To characterize coherent structures in the case of Homogeneous Isotropic Turbulence (HIT) with no density variation, we can define several important metrics. The two-point correlation function, for instance, is defined as,

$$R_{\phi\psi}(\xi,t) = \langle \psi'(\underline{x},t)\phi'(\underline{x}+\xi,t)\rangle, \qquad (4.353)$$

where $\langle \cdot \rangle$ is the averaging operator over the homogeneous direction. We can also consider the longitudinal velocity correlation coefficient,

$$f(\xi,t) = \frac{3}{2\kappa} R_{11}(\xi \hat{\underline{n}}_1, t) = \frac{\langle u_1'(\underline{x}, t) u_1'(\underline{x} + \xi \hat{\underline{n}}_1, t) \rangle}{\langle u_1' u_1' \rangle},$$
(4.354)

and the transverse velocity correlation coefficient,

$$g(\xi, t) = \frac{3}{2\kappa} R_{22}(\xi \underline{\hat{n}}_1, t) = \frac{\langle u'_2(\underline{x}, t) u'_2(\underline{x} + \xi \underline{\hat{n}}_1, t) \rangle_x}{\langle u'_1 u'_1 \rangle_x}.$$
(4.355)



FIGURE 4.34 Filter profiles in spectral space.

Note that the correlation coefficient is simply the normalized correlation function:

$$f_{\psi,\phi} = \frac{\langle \psi'(\underline{x},t)\phi'(\underline{x}+\xi\hat{\underline{n}}_1,t)\rangle_x}{\sqrt{\langle \psi'^2(\underline{x},t)\rangle\langle \psi'^2(\underline{x}+\xi\hat{\underline{n}}_1,t)\rangle}}.$$
(4.356)

Let us now consider spatial scales that can be derived from the velocity correlation coefficient (i.e. the longitudinal autocorrelation):

$$R_{ij}(\underline{r},t) = \langle u_i(\underline{x},t)u_j(\underline{x}+\xi\hat{\underline{n}}_1,t)\rangle_x.$$
(4.357)

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FIGURE 4.35 Two-point correlation coefficients in axial direction (dashed line) and along the stoichiometric surface (solid lines) for different quantities.

With this, the integral scales defining larger eddies in the flow can be evaluated by integrating the longitudinal and transverse autocorrelations from Eq. (4.354) and Eq. (4.355):

$$L_{11}(t) = \int_{0}^{\infty} f(\xi, t) d\xi$$
 (4.358)

$$L_{22}(t) = \int_0^\infty g(\xi, t) d\xi.$$
 (4.359)

The Taylor microscale is between the integral scale and the Kolmogorov scale $(L \lambda \eta)$, but does not have a clear physical interpretation,

$$\lambda_f(t) = \left(-\frac{1}{2}\frac{\partial^2 f}{\partial\xi^2}(0,t)\right)^{-1/2}$$
(4.360)

$$\lambda_g(t) = \left(-\frac{1}{2}\frac{\partial^2 g}{\partial\xi^2}(0,t)\right)^{-1/2} \equiv \frac{1}{\sqrt{2}}\lambda_f \tag{4.361}$$

By introducing these scales, we can define the following relations:



FIGURE 4.36 Spatial evolution of integral length scales in axial direction (dotted lines with circles) and along the stoichiometric surface (solid lines with symbols). The solid and dotted lines correspond to the regression lines.

	Integral Scale	Taylor Scale	Kolmogorov Scale
Length	$L_u = \frac{k^{3/2}}{\epsilon}$	$\lambda_g = \left(10\frac{k\nu}{\epsilon}\right)^{1/2}$	$\eta = \left(\frac{\nu^3}{\epsilon}\right)^{1/4}$
Time	$ au_u - rac{k}{\epsilon}$	$\tau_{\lambda} = \left(15\frac{\nu}{\epsilon}\right)^{1/2}$	$\tau_{\eta} = \left(\frac{\nu}{\epsilon}\right)^{1/2}$
Velocity	$u_u = k^{1/2}$	$u_{\lambda} = \left(\frac{2}{3}k\right)^{1/2}$	$u_{\eta} = (\epsilon \nu)^{1/4}$
Turbulent Reynolds Number	$Re_L = \frac{k^2}{\epsilon\nu}$	$Re_{\lambda} = \frac{u'\lambda_g}{\nu}$	$Re_{\eta} = 1$

TABLE 4.31 Turbulent scales.

- Turbulent Kinetic Energy: $k = \frac{1}{2}\overline{u'_i u'_i} = \frac{1}{2}\sum_i \overline{u''_i}^2$ Turbulent Dissipation Rate: $\epsilon = \nu \overline{\partial_k u'_i \partial_k u'_i} = 2\nu \overline{S_{ij} S_{ij}}$

For the description of turbulent flows, we can introduce the following scales: Other important relations include,



FIGURE 4.37 Comparison of computational results and experimental data for hydroxyl radical correlation (a) two-point correlation coefficient and (b) integral length scale. The dotted line in (a) shows the location where $(\widetilde{Z}) = Z_{\rm st}$.



Separation Distance, ξ

FIGURE 4.38 Change in correlation with separation distance.

- Ratio of Transverse Taylor Microscale to Turbulence Integral Scale: $\frac{\lambda_g}{L_u} \simeq \sqrt{10} R e_L^{-1/2}$ Ratio of Kolmogorov and Turbulent Integral Scales: $\frac{\eta}{L_u} = R e_L^{-3/4}$

• Taylor Scale Reynolds Number: $Re_{\lambda} = \frac{u'\lambda_g}{\nu} = \left(\frac{2}{3}k\right)^{1/2} \frac{\lambda_g}{\nu} = \left(\frac{20}{3}Re_L\right)^{1/2}$ Integral time scales are evaluated in analogy using auto-correlation function:

$$\rho_{ij} = \frac{\langle u'_i(\underline{x},t)u'_j(\underline{x},t+\zeta)\rangle}{\langle u'_iu'_j\rangle}$$
(4.362)

$$\tau = \int_0^\infty \rho(t)dt. \tag{4.363}$$

4.3.5. Turbulence Energy Spectrum. For homogeneous turbulence, we can introduce the velocity spectrum tensor $\underline{\Phi}$, which is related to the Fourier transformation of the two-point autocorrelation function.

$$\underline{\underline{\Phi}}_{ij}(\underline{\kappa},t) = \frac{1}{(2\pi)^3} \iiint_{-\infty}^{\infty} R_{ij}(\underline{\xi},t) \exp\{-i\underline{\kappa} \cdot \underline{\xi}\} d\underline{\xi}$$
(4.364a)

$$R_{ij}(\underline{\xi}, t) = \iiint \phi_{ij}(\underline{\kappa}, t) \exp\left\{-\underline{\kappa} \cdot \underline{\xi}\right\} d\kappa$$
(4.364b)

Using this result, Reynolds stresses are obtained for $\xi \to 0$ as,

$$R_{ij}(0,t) = \langle u_i u_j \rangle = \iiint_{-\infty}^{\infty} \Phi_{ij}(\underline{\kappa},t) d\underline{\kappa}.$$
(4.365)

Additionally, the definition of the turbulent kinetic energy spectrum can be useful in modeling and analysis of turbulence,

$$E_i(\kappa, t) = \frac{1}{2} \iiint_{-\infty}^{\infty} \Phi_{ii}(\underline{\kappa}, t) \delta(\kappa - |\underline{\kappa}|) d\underline{\kappa}.$$
(4.366)

For isotropic turbulence, the velocity spectrum tensor is related to the turbulent energy spectrum:

$$\underline{\underline{\Phi}}_{ij}(\underline{\kappa},t) = \frac{E_u(\kappa,t)}{4\pi\kappa^2} \left(\delta_{ij} - \frac{\kappa_i \kappa_j}{\underline{\kappa}^2} \right).$$
(4.367)

The turbulent kinetic energy is thus,

$$k(t) = \int_0^\infty E_u(\kappa, t) d\kappa = \frac{1}{2} \langle u'_i u'_i \rangle.$$
(4.368)

and the turbulent energy dissipation is,

$$\epsilon(t) = 2\nu \int_0^\infty E_u(\kappa, t) \kappa^2 d\kappa.$$
(4.369)



FIGURE 4.39 Turbulence energy spectrum.

4.3.6. Model Velocity Spectrum. It is convenient to model the turbulence energy spectrum of several key reasons:

- To provide initial conditions for DNS
- Closure for turbulence model (e.g. rapid distortion theory)
- Estimate energy at smallest scales
- Comparison with experiments

Example of model spectra include:

• Pao Spectrum:

$$E(\kappa) = \alpha \epsilon^{2/3} \kappa^{-5/3} \exp\left(-\frac{3\alpha}{2} \kappa^{1/3}\right)$$
(4.370)

• Von Karman Spectrum:

$$E(\kappa) = \alpha \epsilon^{2/3} L^{5/3} \frac{L^4 \kappa^4}{(1 + L^2 \kappa^2)^{17/6}}$$
(4.371)

• Pope:

$$\frac{18}{55}K_0\epsilon^{2/3}\kappa^{-5/3} \tag{4.372}$$

• Passot-Pouquet Spectrum:

$$E(\kappa) = \frac{16\overline{u'^2}}{\kappa_e} \sqrt{\frac{2}{\pi}} \left(\frac{\kappa}{\kappa_e}\right)^4 \exp\left\{-2\left(\frac{\kappa}{\kappa_e}\right)^2\right\}$$
(4.373)

with $u' = \sqrt{2k/3}, \ \kappa_e = 2\pi/L_u$

The general form of the spectrum can be written as:

$$E_u(\kappa) = C\epsilon^{2/3}\kappa^{-5/3}f_L(\kappa L_u)f_\eta(\kappa\eta), \qquad (4.374)$$

where f_L and f_η are cutoff functions, $f_L \sim \kappa^{\gamma}$, $f_\eta = \exp\{-(\kappa\eta)^{\alpha}\}$, $\alpha \sim 4$, and $\gamma = 2...4$.

Discussion Box 9: Combustion Noise in Turbulent Flames

One of the key issues in practical combustion systems is the emission of large amounts of noise. In fact, due to significant reduction in hydrodynamic jet noise and anticipated advancements in the noise suppression of turbomachinery, combustion noise is becoming a leading contributor to the overall aircraft noise emission, and is now considered as a lower aircraft noise limit. Furthermore, advanced combustion concepts, such as rich-quench-lean combustors, staged fuel injection systems, and lean premixed prevaporized combustion can lead to considerable increase in noise emissions. The main reasons for this are that lean premixed and stratified combustion modes are receptive to combustion-driven oscillations, and spatially inhomogeneous heat release and turbulence fluctuations can amplify the noise generation in staged combustion (such as the integral scale and two-point correlation) to arrive at key insights about the turbulent and scalar structures in a reacting flowfield simulated via LES. Thus, these fundamentals of turbulent combustion are not merely academic definitions – they often represent key points of analysis and comparison in assessing flows a manner that can have direct impact on the design of practical systems such as aircraft engines.

4.4. Description of Scalar Turbulent Mixing and Scales of Scalar Mixing

4.4.1. Phenomenological Description. Here we will only focus on conserved scalars. A conserved scalar refers to a quantity that is neither consumed nor produced, and therefore does not contain a source term in its transport equation. In contrast, a passive scalar is a scalar that does not affect the flow field. For the case of constant density, a conserved scalar is identical to a passive scalar.

$$D_t \phi = \alpha \nabla^2 \phi, \tag{4.41}$$

or

$$D_t \phi = \frac{1}{ReSc} \nabla^2 \phi \tag{4.42}$$

where $Sc = \nu/\alpha$ is the Schmidt number describing the ratio of kinematic viscosity to molecular species diffusivity. To describe scalar mixing, we can introduce two scales:

(1) Scalar Integral Scale:

In analogy to the inertial velocity scale L_u defined in Tab. 4.31, this scalar integral scale. L_{ϕ} , characterizes the largest structures in a scalar field. The evolution of L_{ϕ} is determined by the combination of initial conditions and turbulent mixing. This length scale is defined as,

$$L_{\phi} = \int_0^{\infty} f_{\phi}(\xi, t) d\xi, \qquad (4.43)$$

with,

$$f_{\phi} = \frac{\langle \phi'(\underline{x}, t) \phi'(\underline{x} + \xi \hat{\underline{e}}_{\xi}, t) \rangle}{\phi'^2}.$$
(4.44)

Remembering that $L_u = k^{3/2}/\epsilon$ and $L_{\phi} = (\alpha/\chi_{\phi})^{1/2}$ with $\chi_{\phi} = 2\alpha |\nabla \phi|^2$, it is important to realize that models for scalar mixing must reproduce the interaction between L_u and L_{ϕ} .

(2) Batchelor Scale:

The Batchelor scale λ_B characterizes the smallest scalar eddies where molecular diffusion is balanced by turbulent mixing,

$$\lambda_B = \frac{1}{\sqrt{Sc}}\eta,\tag{4.45}$$

This expression which is obtained by recognizing,

$$Sc = \frac{\nu}{\alpha} \sim \frac{\eta^2 / \tau_{\eta}}{\lambda_B^2 / \tau_{\phi}},\tag{4.46}$$

and setting the timescales τ_{η} and τ_{ϕ} equal. Note that for gaseous combustion, $Sc \sim 1$, while $Sc \sim 1000$ for liquids [18].



FIGURE 4.41 Effect of Schmidt number on Batchelor scale.

A few observations are now in order. First, while $Sc \sim 1$ in gas-phase flows, in the liquid phase $Sc \gg 1$ in general, as the scalar field contains fine-scale structures at scales smaller than the velocity field. Further, from a physical standpoint, when $l_{\phi} \gg \lambda_B$, molecular diffusion is negligible and an initially non-premixed field will remain segregated. The important implication here is that for turbulent reacting flows, the chemical source term will be coupled to turbulent mixing. At high Reynolds numbers in particular, the small scales of the scalar fields are isotropic, and evolve on timescales that are short compared to the large scales. Indeed, the characteristic timescales for mixing when $l_{\phi} > \lambda_B$ are fully determined by the turbulent flow.

As a result, as $Sc \to \infty$, Eq. (4.41) reduces to the equation,

$$\partial_t \phi + \underline{u} \cdot \nabla \phi = 0, \tag{4.47}$$

as turbulence only changes the length-scale distribution (or the scalar energy spectrum). With $\alpha \neq 0$, we have slow mixing, and stratified ligaments or lamella structures can form, as schematically illustrated in Fig. 4.41.





We can now estimate the scalar mixing rate γ from the spectral energy transfer,

$$\gamma(l_{\phi}) = \frac{1}{\tau_{\phi}} \left(\frac{L_{\phi,0}}{l_{\phi}}\right)^{2/3} \left[\frac{1}{s}\right], \qquad (4.48)$$

where τ_{ϕ} is a turbulent mixing time and $L_{\phi,0}$ is the initial scalar length scale. We can consider large-scale (i.e. integral-scale) mixing in a similar fashion. In this case, $l_{\phi} = L_u$, $\tau = \tau_u = k/\epsilon$, and $L_{\phi,0} = L_u$. Thus, we have,

$$\gamma(L_u) = \frac{\epsilon}{k} \tag{4.49}$$

We can also consider mixing in the inertial range (Kolmogorov mixing), where,

$$\gamma(\eta) = \left(\frac{\epsilon}{\nu}\right)^{1/2} = Re_L^{1/2}\gamma(L_u); \quad l_\phi \le \eta, \tag{4.410}$$

with $\tau_{\eta} = \left(\frac{\nu}{\epsilon}\right)^{1/2}$. Finally, for the inertial subrange, we have,

$$\gamma(l_{\phi}) = \frac{1}{\tau_{\eta}} \left(\frac{\eta}{l_{\phi}}\right)^{2/3}, \quad \eta \le l_{\phi} \le L_u$$
(4.411a)

$$= \left(\frac{\epsilon}{\nu}\right)^{1/2} \left(\frac{\eta}{l_{\phi}}\right)^{2/3} \tag{4.411b}$$

At high Reynolds numbers, Kolmogorov mixing is much faster than integral scale mixing, but overall mixing is controlled by integral scale mixing (i.e. integral scale mixing is rate-limiting). The mixing time t_{mix} can then be defined as,

$$l_{\phi}(t=0) = L_{\phi} \to l_{\phi}(t_{mix}) = \lambda_B. \tag{4.412}$$

A simple mixing model can then be developed to evaluate t_{mix} ,

$$\frac{\partial l_{\phi}}{dt} = -\gamma(l_{\phi})l_{\phi} \tag{4.413}$$

(4.414)

Denoting t_K as the time required for l_{ϕ} to reduce from L_{ϕ} to η , we can use Eq. (4.413) and Sec. 4.4.1 to write,

$$t_K = \frac{3}{2} \left[\left(\frac{L_\phi}{\eta} \right)^{2/3} - 1 \right] \tau_\eta, \qquad (4.415)$$

$$= \frac{3}{2} \left(\frac{L_{\phi}}{L_{u}}\right)^{2/3} \tau_{u} - \frac{3}{2} \tau_{\eta}.$$
(4.416)

At high Reynolds numbers, $\tau_\eta \ll \tau_u$, meaning that,

$$t_K \approx \frac{3}{2} \left(\frac{L_\phi}{L_u}\right)^{2/3} \tau_u \tag{4.417}$$

In similar fashion, letting t_B denote the time required for l_{ϕ} to reduce from η to λ_B , we find that,

$$t_B = \frac{1}{2} ln(Sc)\tau_\eta, \qquad (4.418)$$

implying that the overall mixing time can be approximated as,

$$t_{mix} \approx \frac{3}{2} \left(\frac{L_{\phi}}{L_u}\right)^{2/3} \tau_u + \frac{1}{2} \ln(Sc)\tau_\eta \tag{4.419}$$

A few quick observations are now in order. First, the effects of the Schmidt number are only relevant for $Sc \gg 1$. Second, the scalar-to-velocity-length-scale ratio L_{ϕ}/L_u is a key parameter in scalar mixing. Third, for the case that $L_{\phi} = L_u$, the mixing time scale is directly controlled by the turbulent flow and $t_{mix} = \tau_u$.

The description of scalar mixing can also be represented using a statistical method. Since the scalar field and the velocity field are directly coupled, it is convenient to introduce a one-point velocity composition PDF,

$$P_{\phi}(\psi) = \int P_{\underline{u},\phi}(\underline{u},\underline{\psi})dV = \frac{P_{\underline{u},\phi}(\underline{v},\underline{\psi})}{P_{\underline{u}|\phi}(\underline{v}|\underline{\psi})},\tag{4.420}$$

with u a random variable and \underline{v} a sample variable. We can consider the binary mixing situation, wherein at $t = t_0$. we have,

$$P_{\phi}(\psi) = \alpha \delta(\psi) + (1 - \alpha)\delta(1 - \psi). \tag{4.421}$$



FIGURE 4.43 Binary mixing PDFs.

In this case, the mean is:

Mean:
$$\langle \phi(x,0) \rangle = \int_0^1 \psi P_{\phi}(\psi) d\psi = \langle \phi(x,t) \rangle$$
 (4.422)

Variance:
$$\langle \phi'^2(x,t) \rangle = \int_0^1 (\psi - \langle \phi \rangle)^2 P_{\phi}(\psi) d\psi.$$
 (4.423)

At this point, we can use P_{ϕ} to drive closure models. For this, consider a generic function $S(\psi)$. We can compute a statistical moments by integrating over P_{ϕ} ,

$$\langle S(x,t)\rangle = \int S(\underline{\psi}) P_{\phi}(\underline{\psi};\underline{x},t) d\underline{\psi}.$$
(4.424)

This closure model is the foundation of presumed PDF models and topology-based combustion models for modeling turbulence-chemistry interaction.

4.4.2. Scalar Energy Spectrum. Similar to the kinetic energy spectrum of Sec. 4.3.6, we can introduce a scalar energy spectrum E_{ϕ} . From the previous analysis, we can anticipate that E_{ϕ} has a similar structure in the inertial range as E_k and, dependent on L_{ϕ} and s_L , will behave differently in the energy-containing and dissipative range. A starting point for understanding this is the definition of a scalar spatial correlation function,

$$R_{\phi}(\underline{\xi},t) = \langle \phi'(\underline{x},t)\phi'(\underline{x}-\underline{\xi},t) \rangle_x, \qquad (4.425)$$

and the scalar spectrum,

$$\Phi_{\phi}(\underline{\kappa},t) = \frac{1}{(2\pi)^3} \iiint R_{\phi}(\underline{\xi},t) \exp\left\{-i\underline{\xi} \cdot \underline{\kappa}\right\} d\underline{\xi}$$
(4.426)

$$R_{\phi}(\underline{\xi}, t) = \iiint \Phi_{\phi}(\underline{\kappa}, t) \exp\left\{i\underline{\xi} \cdot \underline{\kappa}\right\} d\underline{\kappa}.$$
(4.427)

With zero-separation $(\xi = 0)$, we obtain the scalar variance,

$$R_{\phi}(0,t) = \langle \phi'^2 \rangle = \iiint \Phi_{\phi}(\underline{\kappa},t) d\underline{\kappa}.$$
(4.428)

The one-dimensional scalar spectrum is,

$$E_{\phi}(\kappa, t) = \iiint \Phi_{\phi}(\underline{\kappa}, t) \delta(|\underline{\kappa}| - \kappa) d\underline{\kappa}.$$
(4.429)

and by introducing a spherical coordinate system, we obtain by transforming,

$$d\underline{\kappa} = \kappa^2 \sin\theta d\kappa d\alpha d\theta \tag{4.430}$$

$$E_{\phi}(\kappa, t) = 4\pi \kappa^2 \Phi_{\phi}(\kappa, t). \qquad (4.431)$$

From this, we can derive some useful definitions within the realm of isotropic turbulence:

• Scalar variance:

$$\langle \phi'^2 \rangle(t) = \int_0^\infty E_\phi(\kappa, t) d\kappa$$
 (4.432)

• Scalar Integral Length Scale:

$$L_{\phi}(t) = \frac{\pi}{2\langle \phi'^2 \rangle} \int_0^\infty \frac{E_{\phi}(\kappa, t)}{\kappa} d\kappa$$
(4.433)

• Scalar Dissipation Rate:

$$\chi_{\phi} = 2\alpha \int_0^\infty \kappa^2 E_{\phi} d\kappa \tag{4.434}$$

• Scalar Mixing Time:

$$\tau_{\phi} = \frac{2\langle \phi'^2 \rangle}{\chi_{\phi}} \tag{4.435}$$

With these definitions, we can introduce a scalar model spectrum. Note that this spectrum is similar to the kinetic energy spectrum, but there are many and different expressions. The most common ones are due to Corrsin, Obuknov, and Batchelor et al. The formulation of E_{ϕ} requires consideration of Schmidt number effects (e.g. for $Sc \gg 1$, $\kappa_B = \sqrt{Sc\kappa_{\eta}}$). The inertial subrange is not affected by viscosity and diffusivity, and will be similar for E_{ϕ} and E_u . Further, the scalar energy-containing range will follow the inertial sub-range. At high Re_L , E_{ϕ} will be dominated by the energy-containing and inertial/inertial-convective sub-ranges. The model scalar energy spectrum can be expressed as,

$$E_{\phi}(\kappa) = C_{OC} \chi_{\phi} \epsilon^{-3/4} \nu^{5/4} (\kappa \eta)^{-\beta(\kappa \eta)} f_L(\kappa L_u) f_B(\kappa \eta), \qquad (4.436)$$

where C_{OC} is the Obukhov-Corrsin constant ($\approx 2/3$) and β is a scaling exponent such that,

$$\beta = f(Sc) = \begin{cases} 5/3 & \text{for } \kappa\eta \to 0\\ 1 & \text{for } \kappa\eta \to \infty \end{cases}$$
(4.437)

and f_L, f_B are cutoff functions. Further,

$$\beta = 1 + \frac{2}{3} \left[7 - 6f_D(\kappa \eta) \right] f_\eta(\kappa \eta)$$
(4.438)

$$d = \frac{1}{2} + \frac{1}{4} f_{\eta}(\kappa \eta), \qquad (4.439)$$

$$f_D = (1 + C_D S c^{-d(\kappa\eta)/2} \kappa \eta) \exp\left\{-C_D S c^{-d(\kappa\eta)/2} \kappa \eta\right\}$$
(4.440)

$$f_B = \exp\left\{-C_d S c^{-2d(\kappa\eta)}(\kappa\eta)^2\right\},\tag{4.441}$$

with f_D the diffusive-scale cutoff function, f_B the Batchelor scale cutoff function, and $C_D = 2.59$. The value of c_d is dependent on Reynolds and Schmidt numbers for Sc < 1, but takes a value of 2 for Sc > 1. More information can be found in [22].



FIGURE 4.44 Illustration of turbulent scalar spectrum.

By comparing the scalar and turbulence time scale, one can introduce the mechanical-to-scalar time scale ratio $C_{\phi},$

$$C_{\phi} = \frac{\tau_u}{\tau_{\phi}} \tag{4.442}$$

$$= \frac{k}{\epsilon} \frac{\chi_{\phi}}{\langle \phi'^2 \rangle}, \tag{4.443}$$

with $\tau_u = k/\epsilon$ and $\tau_{\phi} = \langle \phi'^2 \rangle / \chi_{\phi}$.

4. TRANSITION AND TURBULENCE



FIGURE 4.45 Effect of Schmidt and Reynolds number on time scale ratio C_ϕ

Discussion Box 10: Turbulent Scalar Transport and Mixing

Even to the present day, the finer points of turbulent scalar transport and mixing remain both important and a topic of significant research. Early work [1] contains a detailed theoretical investigation of the form of the scalar spectrum for temperature, taking into account the effects of both convection and molecular diffusion. From these results, the dominant feature of the action of the turbulent motion on the temperature distribution is a continuous reduction of the length-scale of temperature variations. The random convection of material elements of the fluid is inevitably accompanied by distortion of these elements, and, in the absence of molecular transport, a (statistical) increase in the gradients of temperature. It is also found that the continuous increase in the magnitude of temperature gradients due to random convection will ultimately be checked by the smoothing action of thermal diffusion, and no further refinement of the temperature distribution can occur; in this way, a length-scale characterizing the smallest temperature 'eddies ' can be determined. Unfortunately for Batchelor, no measurements were available for comparison with the theoretical results.

In recent years, the advent of laser diagnostics has enabled the scientific community to learn a great deal more about turbulent scalar transport. The work of [12] and [1], for instance, demonstrates remarkable visualizations of layer-like fine structures in high Reynolds number flows. The resolution achieved is finer than the local strain-limited molecular diffusion scale, allowing the fine structure of $Sc \gg 1$ molecular mixing in turbulent flows to be directly determined. Note that due to the high Schmidt number, these flows were often inaccessible to Direct Numerical Simulation (DNS) at the time these studies were performed.

Perhaps the most interesting result of these studies is the fact that the sparseness of the scalar energy dissipation field indicates that a very small proportion of the flow is responsible for a very large proportion of the mixing, implying that there may be a way to engineer more effective mixing via direct utilization of turbulent mixing structures. Further, the demonstration that the fine-scale mixing structures are asymptotically independent of Reynolds number in the high-Reynolds-number limit is fundamentally interesting in light of asymptotic theory about turbulent mixing.

Even more recently, fundamental problems in turbulent scalar mixing have become accessible to simulation. The work of [11], for instance, uses an LES-based method to numerically study passive-scalar mixing by a turbulent shear flow at high Schmidt number (Sc = 1024). This work was originally intended to address inconsistencies between previous studies concerning the formation of power-law scaling in the scalar-energy spectra at viscous-convective scales. Importantly, the scalar timeseries and spatial data reported in this work produced the first power spectra from a LES shear-flow study that exhibits κ^{-1} scaling at viscous-convective scales originally predicted by [4] and consistent with DNS of simpler $Sc \gg 1$ flows.

CHAPTER 5

Fundamentals of Combustion Modeling

To study turbulent combustion, it is instructive to review the asymptotic flame structure of two flames:

- (1) **Premixed Flames**: Fuel and air are mixed prior to combustion
- (2) Diffusion/Non-premixed Flames: Fuel and oxidizer are separated

5.1. Activation Energy

Combustion is controlled by chemical reactions, which have large activation energy barriers. Consider, for instance, the exothermic reaction,

$$A + B \to C + D. \tag{5.11}$$

as diagrammed in Sec. 5.1.



Reaction Coordinate

FIGURE 5.11 Activation Energy Diagram.
The activation energy E_A is typically much larger than temperature change due to heat release,

$$\frac{E_A}{\mathcal{R}T_b} = \frac{T_A}{T_b},\tag{5.12}$$

where T_A is the activation temperature and T_b is the characteristic flame temperature. In the large activation energy limit, this implies,

$$\frac{T_A}{T_b} = Ze \gg 1. \tag{5.13}$$

Since the chemical reaction rate is a function of T_A/T ,

$$w = k_f [\mathbf{A}_i]^{\nu'_i}; \quad k_f = AT^\beta \exp\left\{\frac{-E_A}{\mathcal{R}T}\right\},\tag{5.14}$$

this implies that the chemical source term is strongly sensitive to temperature,

$$w \sim \exp\left\{-\frac{T_A}{T}\right\} \rightarrow \frac{\partial w}{\partial T} = \left(\frac{T_A}{T}\right)\frac{w}{T}.$$
 (5.15)

By expanding the exponential source term,

$$w \sim \exp\left\{-\frac{T_A}{T}\right\} = \exp\left\{-\frac{T_A}{T_b}\left(\frac{T_b}{T} + 1 - 1\right)\right\}$$
(5.16)

$$= \exp\left\{-\frac{T_A}{T_b}\right\} \exp\left\{-\frac{T_A}{T_b}\left(\frac{T_b - T}{T}\right)\right\}$$
(5.17)

$$= \exp\left\{-Ze\right\} \exp\left\{-ZeCe\right\},\tag{5.18}$$

where we recall that $Ze \sim O(10)$ and $Ce \sim O(1)$. As a result of the large activation energy and strong temperature sensitivity of reaction rates, flames are confined to thin regions of $O(10 \ \mu\text{m})$. In the reaction zone, the temperature is sufficiently high and the residence time is long enough so that there is sufficient time for reactants to converted by the chemical reaction. Because of similarity with thin boundary layer theory, different analytic methods have been developed to study flame characteristics in the asymptotic limit:

- Damköhler number asymptotics [DNA] (Fendell, Williams), e.g. [21]
- Large activation energy asymptotics [AEA] (Zeldovich, Liñnán, Buckmaster & Williams), e.g. [40]
- Rate-ratio asymptotics [RRA], e.g. [47]

The results of DNA were the basis for flamelet models in turbulent combustion, while AEA considers single step chemistry and RRA considers a multi-step chemistry mechanism to characterize flame structure.

5.2. A Reduced Methane-Air Reaction Mechanism

Of fundamental importance to combustion is methane oxidation, representing the simplest hydrocarbon fuel. Detailed methane pathways can be separated into C1 and C2 low temperature pathways with initial temperatures between 300K and 700K [64]. Sec. 5.2 gives a schematic overview of a reduced methane reaction mechanism.



FIGURE 5.21 Reduced reaction pathways for methane.

A reduced 4-step reaction mechanism derived by Peters and Williams [47] is obtained by invoking the following assumptions:

- Steady state for O, OH, HO₂, CH₃, CH₂O, and CHO.
- Partial equilibrium

Development of the reaction mechanism can be summarized as follows:

(1) Fastest reactions in the C1-chain:

$$CH_4 + H \rightarrow CH_3 + H_2$$
 (R11)

$$CH_3 + O \rightarrow CH_2O + H$$
 (R13)

$$CH_2O + H \rightarrow CHO + H_2$$
 (R17)

$$\underline{\text{CHO} + \text{M}} \rightarrow \underline{\text{CO} + \text{H}} + \underline{\text{M}}$$
(R22)

$$CH_4 + O \rightarrow CO + 2H_2$$
 (A)

(2) Taking partial equilibrium for:

$$H + OH \rightleftharpoons O + H_2 \tag{5.21}$$

$$\underline{\mathrm{H}} + \underline{\mathrm{H}}_{2}\underline{\mathrm{O}} \rightleftharpoons \underline{\mathrm{CO}}_{+}\underline{\mathrm{H}}$$
(5.22)

$$2H + H_2O \rightleftharpoons O + 2H_2 \tag{RB}$$

Combining reactions Eq. (A) and Eq. (RB) gives,

_

$$CH_4 + 2H + H_2O \rightleftharpoons CO + 4H_2$$
 (RI)

(3) Combine the following reactions:

$$\rm CO + OH \rightleftharpoons \rm CO_2 + H$$
 (5.23)

$$H + H_2 O \rightleftharpoons OH + H_2 \tag{5.24}$$

Total:
$$CO + H_2O \rightleftharpoons CO_2 + H_2$$
 (II)

(4) Combine the following reactions:

$$O_2 + H + M \rightarrow HO_2 + M$$
 (R5b)

$$9 \text{ OH} + \text{H}_2\text{O} \rightharpoonup \text{H}_2\text{O} + \text{O}_2 \tag{R9}$$

$$\underline{\mathbf{H} + \mathbf{H}_2 \mathbf{O}} \rightarrow \mathbf{O} \mathbf{H} + \mathbf{H}_2 \tag{R3b}$$

Total:
$$2H + M \rightarrow H_2 + M$$
 (RIII)

(5) Combine the following equations:

$$O_2 + H \rightleftharpoons OH + O$$
 (R1)

$$O + H_2 \rightleftharpoons OH + H$$
 (R2)

$$\underline{OH + H_2} \rightleftharpoons H_2O + H (2x) \tag{R3}$$

Total:
$$O_2 + 3H_2 \rightarrow 2H + 2H_2O$$
 (RIV)

5.3. PREMIXED FLAME STRUCTURE

By combining these results, we obtain a four-step mechanism:

$$CH_4 + 2H + H_2O \rightarrow CO + 4H_2$$
 (Propagation) (RI)

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$
 (Water-Gas Shift) (RII)

$$2H + M \rightarrow H_2 + M$$
 (Recombination/Termination) (RIII)

$$O_2 + 3H_2 \rightarrow 2H + 2H_2O$$
 (Branching) (RIV)

Rate coefficients for reactions I-IV are obtained from the following reaction sequence:

$$CH_4 + H \rightarrow CH_3 + H_2$$
 (RI-11)

$$CO + OH \rightleftharpoons CO_2 + H$$
(RII-10)
$$H \downarrow H \bigcirc \Box \downarrow OH \downarrow H$$
(RII-20)

$$\mathbf{H} + \mathbf{H}_2\mathbf{O} \rightleftharpoons \mathbf{O}\mathbf{H} + \mathbf{H}_2 \tag{R11-3}$$

$$H + O_2 + M \rightarrow HO_2 + M$$
 (RIII-5)

$$H + O_2 \rightharpoonup OH + O \tag{RIV-1}$$

5.3. Premixed Flame Structure

5.3.1. General Characteristics of Methane Flames. In a premixed flame, fuel and oxidizer are mixed prior to entering the combustion chamber. Premixing can only be facilitated below a certain temperature, known as the cross-over temperature (T_c) , so that branching reactions are negligible. Example applications include Bunsen burners, lean premixed gas turbine combustors, and spark ignition engines.



FIGURE 5.31 Bunsen flame diagram.

A one-dimensional representation of premixed flame structure is obtained by considering an unstrained planar flame.



FIGURE 5.32 Planar flame structure.



FIGURE 5.33 1-D calculation results for a premixed flame at $\Phi = 1.0$. Observe the relative thicknesses of the inner and secondary layers.

Note that there are several key definitions here:

- Flame Thickness: $\delta_L = \frac{\alpha}{s_L^0}$ (5.31)
- Inner Layer Thickness: $O(\delta)$ (5.32)
- Outer Layer Thickness: $O(\epsilon)$ (5.33)
 - Preheat Region: O(1) (5.34)

5.3. PREMIXED FLAME STRUCTURE

As a specific example, we can further examine the flame structure of a lean methaneair flame. A diagram of flame structure can be found in Fig. 5.32 while analogous 1-D calculation results are presented in Fig. 5.33 We can interpret the flame structure by considering the reduced four-step reaction sequence of Eq. (RI) - Eq. (RIV).

• Inner (Fuel-Consumption) Layer: Fuel is attacked by H radicals via the propagation reaction of Eq. (RI). H radicals are formed through the branching path Eq. (RIV). A characteristic cross-over temperature T_c can be identified through competition between branching and chain termination:

$$O_2 + H \rightleftharpoons OH + O$$
 (Branching) (R1)

$$O_2 + H + M \rightarrow HO_2 + M$$
 (Termination) (R5)

$$CH_4 + H \rightarrow CH_3 + H_2$$
 (Termination/Propagation) (R11)

The cross–over temperature is typically around 500K larger in methane systems compared to hydrogen-oxygen systems, which helps to explain the low reactivity of methane oxidation. The thickness of the inner layer is estimated from asymptotics as:

$$l\delta \sim \delta \cdot \delta_L \sim 0.1 \cdot 200 \mu m \sim 20 \mu m,$$
 (5.35)

which decreases with increasing pressure $(\delta \sim p^{-1})$

• Oxidation Layer: The oxidation layer is controlled by the water-gas shift reaction of Eq. (RII), the termination reaction of Eq. (RIII), and the branching reaction of Eq. (RIV) reactions. These reactions involve oxidation of CO to CO_2 and H_2 oxidation to H_2O . The thickness of the oxidation layer is:

$$l_{\epsilon} \sim \epsilon \delta_L \sim 3l_{\delta} \sim 60 \mu \mathrm{m}; \ \epsilon \simeq 0.3.$$
 (5.36)

5.3.2. Asymptotic Flame Structure Analysis. Let us now consider a planar unstrained flame under the assumption of unity Lewis number and one-step reaction chemistry, schematically shown in Fig. 5.34. This is the same configuration presented in Fig. 5.33; the derivation is due to Zeldovich, Frank-Kamenetski, and Von Karman.

Reaction chemistry is represented by a first-order irreversible reaction,

$$F + O \rightarrow P,$$
 (5.37)

with reaction rate $\dot{m}_F = \rho Y_F A \exp\left\{-\frac{E_A}{\mathcal{R}T}\right\}$. We utilize the following assumptions:

- Stationary flow with respect to the flame location
- Unity Lewis number Le = 1
- Low Mach number deflagration (p = const)
- Calorically perfect gas $(c_p = \text{const})$



FIGURE 5.34 1D Flame Diagram.

The governing equations of Sec. 2.6.4 can thus be rewritten as:

$$d_x(\rho u) = 0 \tag{5.38}$$

$$\rho s_L^0 d_x Y_f = d_x (\rho \alpha d_x Y_F) - \rho Y_F A \exp\left\{-\frac{E_A}{\mathcal{R}T}\right\}$$
(5.39)

$$\rho s_L^0 d_x T = d_x \left(\frac{\lambda}{c_p} d_x T\right) + \frac{\rho Q Y_F A}{c_p} \exp\left\{-\frac{E_A}{\mathcal{R}T}\right\},\tag{5.310}$$

where Q is the heat release. By combining conservation equations for species and temperature, we can obtain a total enthalpy equation

$$H = \frac{Y_F}{Y_{F,u}} + \frac{c_p(T - T_u)}{QY_{F,u}}$$
(5.311)

with transport equation,

$$\rho s_L^0 d_x H = d_x (\rho \alpha d_x H) \tag{5.312}$$

By introducing the non-dimensional fuel mass-fraction and temperature:

$$Y = \frac{Y_F}{Y_{F,u}} \text{ and } \Theta = \frac{c_p}{QY_{F,u}}(T - T_u), \qquad (5.313)$$

5.3. PREMIXED FLAME STRUCTURE

we can write,

$$H = Y + \Theta. \tag{5.314}$$

Boundary conditions are then:

$$x \to -\infty : H = 1; \quad \Theta = 0, Y = 1 \tag{5.315}$$

$$x \to +\infty : H = 1; \quad \Theta = 1, Y = 0 \tag{5.316}$$

A transformation of coordinate systems,

$$\xi = \int_0^x \frac{\rho s_L^0}{\lambda} dx = \int_0^x \frac{s_L^0}{\alpha} dx; Le = \frac{\lambda}{c_p \rho \alpha},$$
(5.317)

where α is the diffusion coefficient. We can rewrite,

$$d_x \frac{d\xi}{dx} d_\xi = \frac{s_L^0}{\alpha} d_\xi; d_x(\rho \alpha d_x) = \frac{\rho s_L^0}{\alpha} d_\xi^2$$
(5.318)

Note that $\delta_L = \alpha/s_L^0$, and the source term can be expressed as,

$$\exp\left\{-\frac{T_A}{T}\right\} = \exp\left\{-\frac{T_A}{T_b}\left(\frac{T_b}{T} + 1 - 1\right)\right\}$$
(5.319)

$$= \exp\left\{-\frac{T_A}{T_b}\left(\frac{T_b}{\Theta(T_b - T_u) + T_u} + 1 - 1\right)\right\}$$
(5.320)

$$= \exp\left\{-\frac{T_A}{T_b}\right\} \exp\left\{-\frac{T_A}{T_b} \left(\frac{(T_b - T_u)(1 - \Theta)}{\Theta(T_b - T_u) + T_u}\right)\right\}$$
(5.321)

$$= \exp\left\{-\frac{Ze}{Ce}\right\} \exp\left\{-\frac{Ze(1-\Theta)}{(1-Ce)(1-\Theta)}\right\}$$
(5.322)

By introducing the burning-rate eigenvalue (a dimensional parameter):

$$\Lambda = \frac{\alpha A}{s_L^{02}} \exp\left\{-\frac{Ze}{Ce}\right\},\tag{5.323}$$

we can rewrite the reduced set of equations as,

$$d_{\xi}\Theta = d_{\xi}^2\Theta + \Lambda Y \exp\left\{-\frac{Ze(1-\Theta)}{1-Ce(1-\Theta)}\right\}, \quad \xi = \frac{x}{s_L^0}$$
(5.324)

$$\Theta + Y = H(=1) \rightarrow Y = 1 - \Theta \tag{5.325}$$

with boundary conditions:

$$\xi \to -\infty : H = 1; \quad \Theta = 0, Y = 1 \tag{5.326}$$

$$\xi \to +\infty : H = 1; \quad \Theta = 1, Y = 0 \tag{5.327}$$

In the following, we consider the parametric limit $Ze \to \infty$ (i.e. activation energy asymptotics), where Ze characterizes the temperature sensitivity of the overall reaction rate. From the following,

$$w = (1 - \Theta) \exp\left\{-\frac{Ze(1 - \Theta)}{1 - Ce(1 - \Theta)}\right\}, \lim_{Ze \to \infty} w \to 0$$
(5.328)

we can consider the specific cases:

(1)

$$\xi \ll 0: d_{\xi} \to 0; (1 - \Theta) \gg \frac{1}{Ze}$$
 (5.329)

Region of of low temperature and frozen chemistry called a $convection\ diffusion\ zone$

(2)

$$\xi \gg 0: \ d_{\xi} \to 0; \ \Theta \to 1; \ Y \to 0 \tag{5.330}$$

This is known as the *post-flame zone*.

(3)

$$\xi Ze \sim O(1): \ (1 - \Theta) = Y \sim \frac{1}{Ze}; \ \Theta \sim \frac{Ze - 1}{Ze}$$
(5.331)

Known as the *reactive-diffusive zone*

Detailed insight can be obtained through balance analysis:

• Convection-diffusion zone: Governing equations reduce to:

$$d_{\xi}\Theta = d_{\xi}^2\Theta$$
, with: $\xi \to -\infty; \Theta = 0$, (5.332)

and exponentially small reaction term. The solution to this equation is simply,

$$\Theta = \exp\{\xi\} \tag{5.333}$$

$$Y = 1 - \exp\{\xi\}, \xi \le 0. \tag{5.334}$$

This region is referred to as the preheat zone, where the thickness of the preheat zone, $\Delta \xi \sim O(1)$, can be written as,

$$\Delta\xi = \int_0^{\delta_L^0} \frac{s_L^0}{\alpha} dx = \frac{s_L^0}{\alpha} \delta_L^0 \tag{5.335}$$

 Reaction-diffusion zone: The region in which (1 − Θ) ~ Ze⁻¹ (reaction term is exponentially not small). We therefore introduce an inner scale variable,

$$\eta = Ze(\xi - \xi_0) \sim O(1) \tag{5.336}$$



FIGURE 5.35 Matched asymptotic analysis.

From this, we can confirm that,

$$\lim_{\mathrm{Ze}\to\infty}\frac{d\eta}{d\xi}\to\infty,\tag{5.337}$$

meaning that the inner layer becomes infinitely thin in the high activation energy limit. We then expand the dependent variable as $Y \sim y/Ze$ by assuming that fuel consumption is O(1/Ze),

$$y = Ze(1 - \Theta) \to \Theta = 1 - \frac{y}{Ze}, \tag{5.338}$$

in the inner layer structure. Further, this implies:

$$d_{\xi} = \frac{d_{\eta}}{d_{\xi}} d_{\eta} = Zed_{\eta}; \ d\Theta = -\frac{1}{Ze} dy$$
(5.339)

$$= \frac{1}{Ze}d_{\eta}y = -d_{\eta}^{2}y + \frac{\Lambda}{Ze^{2}}y\exp\left\{-\frac{y}{1-\frac{Ce}{Ze}y}\right\}.$$
(5.340)

Further, $Ze \to \infty$ requires that $\frac{\Lambda}{Ze^2} \sim O(1)$, giving the expansion,

$$\Lambda = Ze^2 [\Lambda_0 + \sum_i Ze^{-i\Lambda_i}].$$
(5.341)

Retaining O(1) terms gives the reaction-diffusion balance (in the limit as $Ze \to \infty$):

$$d_{\eta}^2 y = \Lambda_i y \exp\{-y\}. \tag{5.342}$$

with conditions $\eta \to \infty : y \to 0$. By matching slopes, such that $d_{\eta}y = C$ at $\eta = 0$., we can rewrite the diffusion reaction equation to eliminate spatial dependence:

$$\frac{dy^2}{d\eta^2} = \frac{dy}{d\eta}\frac{d}{d_y}\left(\frac{dy}{d\eta}\right) = \frac{1}{2}\frac{d}{dy}\left(\frac{dy}{d\eta}\right)^2.$$
(5.343)

With this, we can rewrite the diffusion equation as,

$$\frac{1}{2}\frac{d}{dy}\left(\frac{dy}{d\eta}\right)^2 = \Lambda_0 y \exp\{-y\},\tag{5.344}$$

and integrate with boundary conditions,

 $\eta \to \infty: y \to 0 \text{ (all fuel is consumed)}$ (5.345)

$$\eta \to -\infty: y \to \infty \text{ (for matching conditions)},$$
 (5.346)

such that,

$$\frac{1}{2} \left(\frac{dy}{d\eta}\right)^2 = \Lambda_0 \int_0^y y' \exp\{-y'\} dy' = \Lambda_0 [1 - \exp\{-y\}(1+y)],$$
(5.347)

where we have used the identity $\int_0^\infty y' \exp\{-y'\} dy' = \Gamma(2) = 1$. At the matching point, we require that,

$$\frac{dy}{d\eta} = C$$
 (Here, we set C = 1), (5.348)

and evaluating the above equation at $\eta \to -\infty \to y \to \infty$ gives,

$$\Lambda_0 = \frac{1}{2} \frac{\Lambda}{Ze^2} \to \Lambda = \frac{1}{2} Ze^2 \tag{5.349}$$

$$\therefore s_L^0 = \left(\frac{2DA}{Ze^2} \exp\left\{-\frac{Ze}{Ce}\right\}\right)^{1/2},\tag{5.350}$$

where we have used the definition of Λ from Eq. (5.323).

Thus, this analysis shows that the flame speed is dependent on the activation energy,

$$\delta_F = \frac{\delta_L^0}{Ze} \tag{5.351}$$

Further, flame speed is a function of equivalence ratio ϕ . The maximum flame speed is obtained at $\phi > 1$ since the heat capacity of the diatomic product gas composition is slightly lower than that characteristic of the lean side.



FIGURE 5.36 Flame speed vs. equivalence ratio.

5.4. Diffusion Flame Structure

5.4.1. General Characteristics of a Diffusion Flame. In a diffusion flame, fuel and oxidizer enter the combustion chamber prior to mixing and combustion. Mixing and combustion are facilitated by a combination of turbulent mixing and molecular diffusion. Chemical reactions take place where reactants are mixed at the molecular level. In terms of relevant timescales,

$$\tau_{Mixing} \gg \tau_{Ch} \to Da = \frac{\tau_{Mixing}}{\tau_{Ch}} \to \infty.$$
 (5.41)

In this framework, it is easily seen that diffusion flames are controlled by molecular mixing and diffusion. Exceptions to this include conditions near extinction, at ignition, and combustion in vitiated flows. Examples of diffusion flames include candles and counterflow/opposed-jet flames

5.4.2. Structure of Diffusion Flames. We now consider the counter-flow diffusion flame, diagrammed in Fig. 5.41. For an analysis of flame structure, we can again use the 4-step reaction mechanism from Eq. (RI) - Eq. (RIV). The outer structure of this diffusion flame is the Burke Schumann solution governed by the overall one step reaction,

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O, \qquad (5.42)$$

with the flame sheet position at $Z = Z_{st}$ The inner structure, on the other hand, consists of a thin H₂ – CO oxidation layer of thickness $O(\epsilon)$ and thin inner layer of thickness $O(\delta)$ on the rich side. Beyond this layer, the flame is chemically inert due to radical consumption by the fuel. Thus, in the rich part of a diffusion flame, there is an upstream preheat zone of premixed fuel and a downstream diffusion zone.



FIGURE 5.41 Counterflow diffusion flame.

5.4.3. Activation-Energy Asymptotics. We now consider the one-step irreversible reaction with non-unity Lewis number,

$$\nu'_{\rm F} \mathbf{F} + \nu'_{\rm O} \mathbf{O} \to \nu''_{\rm P} \mathbf{P}. \tag{5.43}$$

We now consider the specific configuration of a counterflow flame, with strain rate $a = 2u_O/L$. For the simplified case of constant density (isothermal flow), we then have a self-similar solution such that,

$$u_r = \frac{ar}{2}, \quad u_y = -ay, \tag{5.44}$$

from the mass conservation equation in axisymmetric coordinates $\partial_y u_y + (1/r)\partial_r (u_r r) = 0.$

In this case, we can write the steady state version of the conservation equations in Sec. 2.6.4 as:

$$\nabla \cdot (\rho \underline{u}) = 0 \tag{5.45a}$$

$$\rho \underline{u} \cdot \nabla Y_{\mathrm{F}} = \nabla \cdot (\rho \alpha_{\mathrm{F}} \nabla Y_{\mathrm{F}}) + W_{\mathrm{F}} \nu_{\mathrm{F}} w \qquad (5.45\mathrm{b})$$

$$\rho \underline{u} \cdot \nabla Y_{\mathcal{O}} = \nabla \cdot (\rho \alpha_{\mathcal{O}} \nabla Y_{\mathcal{O}}) + W_{\mathcal{O}} \nu_{\mathcal{O}} w$$
(5.45c)

$$\rho \underline{u} \cdot \nabla Y_{\mathrm{P}} = \nabla \cdot (\rho \alpha_{\mathrm{P}} \nabla Y_{\mathrm{P}}) + W_{\mathrm{P}} \nu_{\mathrm{P}} w \qquad (5.45\mathrm{d})$$

$$\rho c_p \underline{u} \cdot \nabla T = \nabla \cdot (\lambda \nabla T) + Q \dot{\omega}; \quad Q = -\sum_{i=1}^{N_s} \rho_i W_i \nu_i, \quad (5.45e)$$

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with $\nu = \nu'' - \nu'$ and the adiabatic flame temperature T_b ,

$$T_b = T_0 - \frac{Q(Y_{\mathrm{F},u} - Y_{\mathrm{F},b})}{\nu_{\mathrm{F}} W_{\mathrm{F}} c_p}.$$
(5.46)

Moving forward, we introduce the following assumptions:

- (1) Constant transport properties
- (2) Constant density in the thermo-diffusive limit
- (3) Equal molecular weight $(W_{\rm F} = W_{\rm O} = W_{\rm P} = W)$
- (4) We consider the reaction $\nu'_{\rm F} = 1$, $\nu'_{\rm O} = \nu$, $\nu'_{\rm P} = \nu + 1$ for simplicity

The conservation equations can then be simplified to,

$$\nabla \cdot \underline{u} = 0 \tag{5.47}$$

$$\rho \underline{u} \nabla Y_{\rm F} = \rho \alpha_{\rm F} \nabla^2 Y_{\rm F} - W w \tag{5.48}$$

$$\rho \underline{u} \nabla Y_{\rm O} = \rho \alpha_{\rm O} \nabla^2 Y_{\rm O} - W \nu w \tag{5.49}$$

$$\rho \underline{u} \nabla T = \rho \alpha_T \nabla^2 T + \frac{Q}{c_p} w \tag{5.410}$$

This leads to the 1-D conservation equations,

$$\rho u_y \frac{dY_F}{dy} = \rho \alpha_F \frac{d^2 Y_F}{dy^2} - W \left(\frac{\rho}{W}\right)^2 A Y_F Y_O \exp\left\{-\frac{T_a}{T}\right\}$$
(5.411)

$$\rho u_y \frac{dY_O}{dy} = \rho \alpha_O \frac{d^2 Y_O}{dy^2} - W \left(\frac{\rho}{W}\right)^2 A Y_F Y_O \nu \exp\left\{-\frac{T_a}{T}\right\}$$
(5.412)

$$\rho u_y \frac{dT}{dy} = \rho \alpha_T \frac{d^2 T}{dy^2} - \frac{Q}{c_p} \left(\frac{\rho}{W}\right)^2 A Y_{\rm F} Y_{\rm O} \exp\left\{-\frac{T_a}{T}\right\}.$$
(5.413)

Before we analyze the diffusion flame structure, we will first derive an expression for the mixture fraction. For this, we consider a one-dimensional problem and introduce the following normalized variables:

$$\hat{y} = \frac{y}{\sqrt{\alpha_T/a}}$$
; (rescale axial distance with shear layer thickness) (5.414)

$$\hat{Y}_{\rm F} = Y_{\rm F}, \quad \hat{Y}_{\rm O} = Y_{\rm O}$$
 (5.415)

$$\hat{\Theta} = (T - T_{u,\text{st}}) \frac{W c_p(\nu+1)}{Q}$$
(5.416)

$$u_y = -ay; \quad u_r = \frac{ar}{2}\Big|_{r=0}; \quad \hat{u}_y = \frac{u_y}{\sqrt{\alpha_T}}.$$
 (5.417)

This leads to the non-dimensional equations,

$$-\hat{y}\frac{d\hat{Y}_{\rm F}}{d\hat{y}} = Le_{\rm F}\frac{d\hat{Y}_{\rm F}}{d\hat{y}^2} - Da\hat{Y}_{\rm F}\hat{Y}_{\rm O}\exp\left\{-\frac{T_a}{T}\right\}$$
(5.418)

$$-\hat{y}\frac{d\hat{Y}_{\rm O}}{d\hat{y}} = Le_{\rm O}\frac{d\hat{Y}_{\rm O}}{d\hat{y}^2} - Da\hat{Y}_{\rm F}\hat{Y}_{\rm O}\nu\exp\left\{-\frac{T_a}{T}\right\}$$
(5.419)

$$-\hat{y}\frac{d\hat{\Theta}}{d\hat{y}} = \frac{d\hat{\Theta}}{d\hat{y}^2} + Da\hat{Y}_{\rm F}\hat{Y}_{\rm O}(\nu+1)\exp\left\{-\frac{T_a}{T}\right\},\tag{5.420}$$

with $Da = \frac{A}{a} (\rho/W)$ and a the strain rate. For equal (and unity) Lewis number, we can define a set of conservation equations for the mixture fraction defined in Eq. (2.34),

$$\hat{y}\frac{dZ}{d\hat{y}} + \frac{d^2Z}{d\hat{y}^2} = 0, \tag{5.421}$$

where Z = 0 in the oxidizer stream as $\hat{y} \to \infty$ and Z = 1 in the fuel stream as $\hat{y} \to -\infty$. The solution to Eq. (5.421) is given as the following,

$$Z = \frac{1}{2} \operatorname{erfc}\left(\frac{\hat{y}}{\sqrt{2}}\right) = \frac{1}{2} \operatorname{erfc}\left(\sqrt{\frac{a}{2\alpha_T}}y\right),\tag{5.422}$$

where the second expression is in dimensional form. With the definition of mixture fraction, we can introduce the scalar dissipation rate:

$$\chi_Z = 2\alpha_Z |\nabla Z|^2; \quad , \tag{5.423}$$

where α_Z is the diffusivity of the mixture fraction. For the 1D case, this becomes,

$$\chi_Z = 2\alpha_Z \left(\frac{dZ}{dy}\right)^2. \tag{5.424}$$

In the self-similar coordinates defined in Eq. (5.414), we can use the definition of the complimentary error function to obtain,

$$\hat{\chi}_Z = 2a \left(\frac{dZ}{d\hat{y}}\right)^2 \tag{5.425a}$$

$$= 2a \left[-\frac{2}{\sqrt{\pi}} \frac{1}{\sqrt{2}} \exp\left\{ -\frac{1}{2} \hat{y}^2 \right\} \right]^2$$
(5.425b)

$$= 2\frac{2a}{\pi}\exp\{-\hat{y}^{2}\}, \qquad (5.425c)$$

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where we set $\alpha_Z = \alpha_T$. For further analysis, it becomes important to recognize that we can rewrite the spatial derivative operators as:

$$\frac{\partial}{\partial \hat{y}} = \frac{\partial}{\partial Z} \frac{\partial Z}{\partial \hat{y}}; \quad \frac{\partial^2}{\partial y^2} = \left(\frac{\partial Z}{\partial \hat{y}}\right)^2 \frac{\partial^2}{\partial Z^2} = \frac{\chi_Z}{2a} \frac{\partial^2}{\partial Z^2}.$$
(5.426)

Thus, for the 1-D advection-diffusion operator, we have:

$$\hat{y}\frac{d}{d\hat{y}} + \frac{d^2}{d\hat{y}^2} = \left(\hat{y}\frac{dZ}{d\hat{y}} + \frac{d^2Z}{d\hat{y}^2}\right)\frac{d}{dZ} + \frac{dZ}{d\hat{y}}\left(\frac{d^2}{dZd\hat{y}}\right)$$
(5.427)

$$= \left(\frac{dZ}{d\hat{y}}\right)^2 \frac{d^2}{dZ^2},\tag{5.428}$$

where the cancellation in the first term occurs due to mixture fraction conservation.

To develop the analysis further, we consider unity Lewis number $(Le_i = Le = 1)$, and rewrite the governing equations,

$$-\hat{y}\frac{d\hat{Y}_{\rm F}}{d\hat{y}} = \frac{d^2\hat{Y}_{\rm F}}{d\hat{y}^2} - Da\hat{Y}_{\rm F}\hat{Y}_{\rm O}\exp\left\{-\frac{T_a}{T}\right\}$$
(5.429)

$$-\hat{y}\frac{d\hat{Y}_{\rm O}}{d\hat{y}} = \frac{d^2\hat{Y}_{\rm O}}{d\hat{y}^2} - Da\hat{Y}_{\rm F}\hat{Y}_{\rm O}\nu\exp\left\{-\frac{T_a}{T}\right\}$$
(5.430)

$$-\hat{y}\frac{d\hat{Y}_{\rm P}}{d\hat{y}} = \frac{d^2\hat{Y}_{\rm P}}{d\hat{y}^2} + Da\hat{Y}_{\rm F}\hat{Y}_{\rm O}(\nu+1)\exp\left\{-\frac{T_a}{T}\right\}$$
(5.431)

$$-\hat{y}\frac{d\hat{\Theta}}{d\hat{y}} = \frac{d^2\hat{\Theta}}{d\hat{y}^2} + Da\hat{Y}_{\rm F}\hat{Y}_{\rm O}(\nu+1)\exp\left\{-\frac{T_a}{T}\right\}.$$
(5.432)

Where boundary conditions are,

$$\hat{y} \to \infty$$
 (Oxidizer): $\hat{Y}_{\rm O} = 1;$ $\hat{Y}_{\rm F} = 0;$ $\hat{\Theta} = 0;$ $\hat{Y}_{\rm P} = 0$ (5.433)

$$\hat{y} \to -\infty$$
 (Fuel): $\hat{Y}_{\rm O} = 0; \quad \hat{Y}_{\rm F} = 1; \quad \hat{\Theta} = 0; \quad \hat{Y}_{\rm P} = 0.$ (5.434)

Now, we can make several useful observations:

(1) By introducing the mixture fraction definition of Eq. (2.33), we have

$$Z = \frac{(\nu \hat{Y}_{\rm F} - \hat{Y}_{\rm O}) + Y_{\rm O,\mathcal{O}}}{\nu \hat{Y}_{\rm F,\mathcal{F}} + \hat{Y}_{\rm O,\mathcal{O}}} = \frac{\nu \hat{Y}_{\rm F} - \hat{Y}_{\rm O} + 1}{\nu + 1} \bigg|_{Z_{\rm st}} = \frac{1}{\nu + 1}$$
(5.435)

(2) Next, from the equivalence of Eq. (5.431) and Eq. (5.432),

$$\hat{Y}_{\rm P} = \hat{\Theta}; \quad \sum_{i=1}^{N_s} \hat{Y}_i = 1$$
(5.436)

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(3) Simplifying the transformation of Eq. (5.426) gives,

$$\frac{d}{d\hat{y}} = \frac{dZ}{d\hat{y}}\frac{d}{dZ}; \quad \hat{y}\frac{d}{d\hat{y}} - \frac{d^2}{d\hat{y}^2} = \chi\frac{d}{dZ^2}$$
(5.437)

Using these results, we can rewrite our problem statement as,

$$\hat{Y}_{\rm O} = (1 - Z_{\rm st})(1 - \hat{\Theta}) + Z_{\rm st} - Z; \quad Y_F = 1 - \Theta - Y_{\rm O}$$
 (5.438)

$$\hat{Y}_{\rm F} = Z - \Theta Z_{\rm st} \tag{5.439}$$

$$-\hat{\chi}\frac{d\hat{\Theta}}{dZ^{2}} = Da(\nu+1)\hat{Y}_{\rm F}\hat{Y}_{\rm O}\exp\{-Ze\}\exp\{-Ze\}\exp\{-\frac{ZeCe(1-\hat{\Theta})}{1-Ce(1-\hat{\Theta})}\},\qquad(5.440)$$

$$Z \in [0,1]; \quad ZeCe = \frac{T_a}{T_{b,\text{st}}} \frac{T_{b,\text{st}} - T_{u,\text{st}}}{T_{b,\text{st}}} = \frac{T_a}{T_{b,\text{st}}} Ce = ZeCe$$
(5.441)

$$Z = \frac{1}{2} \operatorname{erfc}\left(\frac{\hat{y}}{\sqrt{2}}\right); \hat{\Theta} = \frac{T - T_{u, \text{st}}}{T_{b, \text{st}} - T_{u, \text{st}}}; \quad T_{b, \text{st}} - T_{u, \text{st}} = \frac{Q}{Wc_p}(\nu + 1)$$
(5.442)

We can now identify three trivial flow regimes:

(1) Frozen Flow: $\beta(1 - \hat{\Theta}) \gg 1$ Eq. (5.440) reduces to,

$$\frac{d^2\Theta}{dZ^2} = 0 \to \hat{\Theta} = f(Z) \tag{5.443}$$

(2) Equilibrium Flow with Zero Oxidizer:

$$\hat{Y}_{\rm O} = 0 \to \hat{\Theta} = \frac{1-Z}{1-Z_{\rm st}} \text{ for } Z \le Z_{\rm st}$$
 (5.444)

(3) Equilibrium Flow with Zero Fuel:

$$\hat{Y}_{\rm F} = 0 \rightarrow \hat{\Theta} = \frac{Z}{Z_{\rm st}} \text{ for } Z \le Z_{\rm st}$$
 (5.445)

Liñán further identified four distinguished burning regimes [40] :

(1) Ignition Regime:

Ignition occurs by an increase in Damköhler number, sufficient to cause temperature variations of O(1/ZeCe) such that $(1 - \Theta) \sim 1/ZeCe$.

(2) Partial Burning Regime:

This is an unstable combustion regime where O(1) leakage of fuel and oxidizer through the flame results in instability. See Fig. 5.43a.



FIGURE 5.42 Equilibrium flow with zero fuel.



(3) **Premixed Flame Regime:**

This condition occurs at or near extinction, where the leakage of one reactant through the flame results in a structure resembling that of a premixed flame. See Fig. 5.43b.

(4) **Diffusion Flame Regime:**

In this region, no reactant leakage occurs to first order, resulting in a flame that resembles the case of the fast chemistry/Burke-Schumann limit.

With this characterization we can generate an "S-shape" solution curve. Note that the Damköhler number in this case can be defined as,

$$Da = \frac{\text{Diffusion Time Through Flame}}{\text{Chemical Time}} = \frac{A}{\chi_Z}.$$
(5.446)



FIGURE 5.44 Damkohler stability plot.

Discussion Box 11: Progress in Knowledge of Flamelet Structure

The "flamelet regime" of combustion has received increasing attention in recent decades due to its relevance to both laminar and turbulent combustion. Importantly, the flamelet regime is a limiting regime of turbulent combustion, as at both high Damköhler numbers both premixed and nonpremixed turbulent flames enter the flamelet regime. As a result, understanding flamelet structure and extinction is of great importance to turbulent combustion. Asymptotic analysis has again proven to be a useful tool in these investigations, as the combination of rate-ratio asymptotics and reduced reaction mechanisms in particular has revealed key scale separations defining internal flamelet structure in both premixed and diffusion flames. Other key considerations have included the effect of the strain rate, curvature, and radiative heat loss on flamelet extinction. Fundamental understanding of this regime has been an important contribution to general turbulent combustion modeling, as flamelet models for turbulent combustion have increased in both popularity and applicability in the last several decades. The reader is referred to the excellent review of Williams for further detail [46]. An excellent reference on diffusion flamelets can be found at the following **link**.

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Discussion Box 12: Lifted Flames In addition to common burner-stabilized and counterflow flames, lifted turbulent flame modes are of practical and theoretical interest. The work of [19] contains an excellent review of stabilization mechanisms in lifted turbulent flames, a regime which is often found in such systems as commercial boilers and direct-injection gasoline engines. Lifted flames are of particular interest because, while relatively simple, their stability is governed by a multitude of complex effects resultant from finite-rate chemistry, turbulence-chemistry interaction, the dynamics of heat release, local extinction, and a variety of other considerations. Even internally, the fact that "holes" can appear within turbulent diffusion flames involves the study of "edge flames," an entirely separate class of flames reviewed by [1].

Fundamentally, there exist many hypotheses about the fundamental reason for lifted flame stabilization. These include the following:

- (1) Premixed Flame Theory: The lifted flame base is premixed and is stabilized because it burns at the local burning velocity
- (2) Critical Scalar Dissipation Concept: Flame stabilization is controlled by the extinction of diffusion flamelets, and thus the lifted turbulent flame stabilizes where the appropriate scalar dissipation rate falls below a critical value
- (3) Turbulent Intensity Theory: Enhanced turbulent burning velocity impacts propagation of the reaction zone
- (4) Large Eddy Concept: flame leading-edge is attached to large eddies and can migrate upstream to a neighboring structure in way that routinely stabilizes the flame on a local scale
- (5) Edge-Flame Concept: Theory assumes that the flame leading edge is partially premixed, and thus that it can propagate upstream counter to the local flowfield.

Results to date generally seem to indicate that the partial premixing and edge-flame theories hold the most potential, with debate continuing on the effect of large-scale structures.

Discussion Box 13: Asymptotic Analysis of Flame Structure

The asymptotic structure of premixed flames has been a subject of study for some time. The analysis presented here for the burning rate eigenvalue problem, for instance, follows that of von Karman [10] from the late 1950's. Similarly, the work of [21] concisely demonstrates the use of matched asymptotics to characterize the structure of premixed flames. These types of fundamental theoretical analyses form the basis of many key results in combustion science.

In later years, asymptotic analysis would also become a powerful tool in understanding the behavior of real combustion systems. The work of [40] uses large activation energy asymptotics and a one-step chemistry assumption on an opposed jet configuration to segment an S curve in Da - T space into frozen ignition, partial burning, premixed flame, and diffusion controlled regimes. Importantly, analytic expressions are able to be obtained for ignition and extinction conditions. Nearly 15 years later, [60] demonstrated that it is not possible to fully describe diffusion flame structure using one-step chemistry, as the difference in reaction speed on the rich side (slow) and lean side (fast) yields a critical time-scale separation that is integral to the accurate description of the asymptotic structure of diffusion flames. It was this work that led to the distinguished limit ordering $\epsilon > \nu > \delta$ of the oxidation layer, water-gas shift layer, and fuel consumption layer.

Such analysis continues to have direct application to combustion systems today. The work of [11] applies large activation energy asymptotic principles to demonstrate that cellular diffusion flames form under near-extinction conditions when the Lewis number sinks below a critical value. Prediction of instabilities in diffusion flames can be more difficult than that in premixed flames due to the existence of two effective Lewis numbers (fuel and oxidizer) and the fact that flame structure qualitatively varies with the Damköhler number. In this work, the spatial scales of the cells in such a flame are predicted to be of the same order as the diffusion length scale, and a stability regime is predicted as a function of both initial mixture strength and Damk ohler number. Agreement with experiments nicely demonstrates the applicability of fundamental asymptotic analysis in understanding the behavior of diffusion flames. An excellent resource on asymptotic analysis can be found at the following link.

CHAPTER 6

Turbulent Combustion Modeling

in this chapter, we will provide a qualitative description of the physics of turbulent combustion. For this, we will consider three important phenomena: stabilization mechanisms of lifted turbulent flames, flame autoignition, and triple flames.

6.1. Ignition of Turbulent Combustion

Ignition is defined as the transition from an unreacted state to a fully or vigorous burning state. There are two key types of ignition: spontaneous/self-ignition (also known as autoignition) and forced/assisted ignition (such as spark ignition). Ignition in a homogeneous flow is a classical combustion problem that involves understanding the effects of the flow field and turbulent scale interaction on ignition. From prior analysis, we expect that both mixing and strain/dissipation will require consideration. Examples of transient ignition processes include spark ignition, re-lighting, and accidental fires. The key governing equation is the energy equation of Sec. 2.6.4, which we rewrite in convenient form below,

$$c_p \rho D_t T = \partial_t p + \nabla \cdot (\lambda \nabla T) + \dot{q}_{HR} + \dot{q}_{EX} - \dot{q}_{RAD}, \qquad (6.11)$$

where \dot{q}_{HR} is heat release, \dot{q}_{EX} is the externally supplied energy, and \dot{q}_{RAD} is heat loss (e.g. by radiation). The ignition criterion for a homogeneous mixture becomes,

$$\partial_t T = \frac{1}{c_p \rho} \left[\frac{1}{r} \partial_r (r \lambda \partial_r T) + \dot{q}_{HR} - \dot{q}_{Rad} \right]$$
(6.12)

$$\dot{q}_{HR} = \dot{Q}; \partial_T \sim \frac{T_b - T_\infty}{R} \tag{6.13}$$

$$d_t T \sim \frac{V}{c_p m} \left[-\lambda \frac{1}{R^2} (2T_\infty - T_b) + \dot{Q} \right].$$
(6.14)

6.1.1. Ignition Classification. There exist several classes of ignition methods that one should consider, namely,

- (1) Jet-Flame Configuration
- (2) Mixing Layer
- (3) Opposed Jet-Flame

(4) Volumetric Compression

Of relevance to autoignition is the primary mixture composition:

- Stoichiometric, $Z_{\rm st}$
- Most reactive, Z_{MR}
- Lean mixture, Z_{Lean}
- Rich mixture, Z_{Rich}

where,

$$Z_{Lean} < Z_{MR} < Z_{\rm st} < Z_{Rich} \tag{6.15}$$

For cold reactants, autoignition occurs at Z_{MR} and at regions of low scalar dissipation rate. Ignition at the most-reactive mixture conditions has a number of distinct characteristics.



FIGURE 6.11 Ignition delay time vs. mixture fraction.

The appearance of the ignition site, for instance, is independent of the turbulence time scale. The ignition time tends to decrease with partial premixing, and is shorter in turbulent than in laminar flows. Finally, the most-reactive mixture depends on both the fuel and oxidizer temperature as well as the activation energy of the reaction. The most-reactive mixture is characterized by a competition between the high temperature of the oxidizer and the reduced fuel concentration due to the exponential dependence of the reaction rate on the temperature.

6.1.2. Assisted Ignition. The ignition process in many burners occurs through assisted ignition, and stability is often achieved via strong swirl or recirculation. There are several distinct ignition phases that can be considered (see Fig. 6.12):

6.1. IGNITION OF TURBULENT COMBUSTION

- (1) **Kernel Generation** of a small flame occurs around a spark due to thermal energy deposition and radical formation
- (2) **Flame expansion** occurs due to local propagation of the flame front and turbulent dispersion of the ignited fluid
- (3) **Flame stabilization** refers to the long-term stabilization of a flame in which the combustion reaction is at steady state



FIGURE 6.12 Ignition process figure.



FIGURE 6.13 Flammability limit figure.

The flammability factor F characterizes the propensity of a mixture to ignite,

$$F = \int_{Z_{Lean}}^{Z_{Rich}} P(Z) dZ.$$
(6.16)

It is at this point useful to directly derive an expression for the most reactive mixture. For simplicity, we consider the case of equal moleculuar weights such that,

$$F + O \rightarrow P$$
 (6.17)

and the reaction rate can be written in simple Arrhenius form,

$$w = A \exp\left\{-\frac{E_A}{\mathcal{R}T}\right\} [F][O], \qquad (6.18)$$

with,

$$Y_{\rm F} = Y_{\rm F,\mathcal{F}}Z\tag{6.19}$$

$$Y_{\rm O} = Y_{\rm O,\mathcal{O}}(1-Z) \tag{6.110}$$

$$T = T_{\mathcal{F}} + (T_{\mathcal{O}} - T_{\mathcal{F}})Z \tag{6.111}$$

$$[X_i] = \frac{Y\rho}{W}.\tag{6.112}$$

Thus, we can rewrite the reaction rate as,

$$w = A \frac{\rho^2}{W^2} \exp\left\{-\frac{E_A}{\mathcal{R}T}\right\} Y_{\rm F} Y_{\rm O}$$
(6.113a)

$$= \frac{p^2}{\mathcal{R}^2} A \frac{1}{T^2} \exp\left\{-\frac{E_A}{\mathcal{R}T}\right\} Y_{\rm F} Y_{\rm O}$$
(6.113b)

$$= \frac{p^{2}A}{\mathcal{R}^{2}} \frac{1}{[T_{\mathcal{F}} + (T_{\mathcal{O}} - T_{\mathcal{F}})Z]^{2}} \exp\left\{-\frac{E_{A}}{\mathcal{R}[T_{\mathcal{F}} + (T_{\mathcal{O}} - T_{\mathcal{F}})Z]}\right\} Y_{\mathrm{F},\mathcal{F}} Y_{\mathrm{O},\mathcal{O}}(1-Z)$$
(6.113c)

$$= \frac{p^2 A}{\mathcal{R}^2} Y_{\mathrm{F},\mathcal{F}} Y_{\mathrm{O},\mathcal{O}} \frac{Z(1-Z)}{[T_{\mathcal{F}} + (T_{\mathcal{O}} - T_{\mathcal{F}})Z]^2} \\ \exp\left\{-\frac{E_A}{\mathcal{R}[T_{\mathcal{F}} + (T_{\mathcal{O}} - T_{\mathcal{F}})Z]}\right\}.$$
(6.113d)

6.2. GOVERNING EQUATIONS AND LOW-MACH FORMULATION

Now, letting $T_A = E_A/\mathcal{R}$, $\beta = T_A/T_F$, and $\zeta_T = T_O/T_F$, we can rewrite this as:

$$w = \left(\frac{p^2}{\mathcal{R}T_{\mathcal{F}}}\right)^2 AY_{\mathrm{F},2}Y_{\mathrm{O},1} \exp\left\{-\frac{\beta}{\mathcal{R}[1+(\zeta_T-1)Z]}\right\} \frac{Z(1-Z)}{[1+(\zeta_T-1)Z]^2}$$
(6.114)

$$= Da \exp\left\{-\frac{\beta}{\mathcal{R}[1+(\zeta_T-1)Z]}\right\} \frac{Z(1-Z)}{[1+(\zeta_T-1)Z]^2}.$$
(6.115)

The most reactive mixture is defined as the limiting value of the mixture fraction as $\partial w/\partial Z \rightarrow 0$, which reduces to the following expression,

$$Z_{MR} = \frac{1}{2} \frac{T_A(\zeta_T - 1) - 2 \pm \sqrt{T_a^2(\zeta_T - 1)^2 + 4\alpha_T^2}}{T_A(\zeta_T - 1) + (\zeta_T^2 - 1)}.$$
(6.116)

Discussion Box 14: Ignition in Turbulent Combustion

The work of [4:] provides an excellent overview of applications, analysis, and current research on turbulent ignition. We provide a brief glimpse into the subject here, but refer the reader to [4i] for a more detailed discussion.

Key applications of forced (or assisted) ignition include jet engine relight and spark-ignition engine, while designed autoignition occurs in diesel engined and scramjets. Ignition in turbulent flows is complicated by the stochastic nature of the underlying mixture fraction fields – while a spark may occur in a flow with a mean composition that will ignite, the spark could be supplied at a time and location wherein the local mixture is outside of the flammability limits. Note that even in premixed flows where composition is relatively consistent, fluctuations in the local strain rate can still make ignition a stochastic phenomenon. In terms of simulating these effects, autoignition tends to be particularly unforgiving from a numerical standpoint, often requiring detailed chemistry and careful specification of numerical parameters. Further, autoignition is not uniform – rather, areas with low local scalar dissipation rates tend to ignite first, a reality which has been consistently observed in DNS. A variety of turbulent combustion models have been applied to the autoignition problem, with transported PDF and flamelet methods showing particular applicability. Understanding these phenomena in turbulent sprays remains an open research question on which there exists relatively little present literature.

6.2. Governing Equations and Low-Mach Formulation

In this section, we focus on turbulent combustion modeling. The starting point is the combustion equations that we derived in Sec. 2.6.4. We now consider low-mach formulation of the governing equations describing conservation of mass, momentum, species, and energy first introduced in Sec. 2.5 with the following assumptions,

- Fourier's Law: $q = \lambda \nabla T$
- Fick's Law for $\overline{\overline{D}}$ iffusion: $j = -\rho \alpha \nabla \underline{Y}$
- Neglect buoyancy

For this, we decompose the pressure into a thermodynamic and a hydrodynamic component.

$$p(\underline{x}, t, M) = p_0(t) + M^2 p_2(\underline{x}, t) + O(M^3)$$
(6.21)

, where p_0 is the thermodynamic pressure and p_2 is the hydrodynamic pressure. After inserting this definition into the governing equations and retaining leading order terms in M, we can decouple the momentum conservation from the other equations:

Mass:
$$\partial_t \rho + \nabla \cdot (\rho \underline{u}) = 0$$
 (6.22a)

Momentum:
$$\partial_t(\rho \underline{u}) + \nabla \cdot (\rho \underline{u} \otimes \underline{u}) = -\nabla p_2 + \nabla \cdot \underline{\sigma}$$
 (6.22b)

Species:
$$\partial_t(\rho \underline{Y}) + \nabla \cdot (\rho \underline{u} \underline{Y}) = \nabla \cdot \underline{j} + \rho \underline{\dot{\omega}}$$
 (6.22c)

Total Enthalpy:
$$\partial_t(\rho h_t) + \nabla \cdot (\rho \underline{u} h_t) = \nabla \cdot q$$
 (6.22d)

EOS:
$$p_0 = \rho RT$$
 (6.22e)

where all quantities without a subscript are of zeroth order in the Mach number. As a reminder, the main benefit of this low-Mach formulation is that it enables a decoupling of the momentum conservation equation, which is now only dependent on the hydrodynamic pressure. By decomposing the pressure, sound waves are filtered out, and pressure and density become decoupled in the following manner:

$$\rho(s, \underline{Y}, p_0 + p') \approx \rho(s, \underline{Y}, p_0) + p' \left(\frac{\partial \rho}{\partial p}\right) \Big|_{S, \underline{Y}, V} , \qquad (6.23)$$

and reconizing that the speed of sound is given as,

$$a = \left(\frac{\partial p}{\partial \rho}\right)\Big|_{S},\tag{6.24}$$

it immediately follows that $a \to \infty$, meaning that the solution will propagate at infinite speed through the medium.

6.3. Favre-Averaging

Applying the Favre-averaging/filtering method described in 4.3.2.2 to the foverning equations with $\phi = \tilde{\phi} + \phi''$ and $\tilde{\phi}$ the filtered quantity allows us to obtain the following set

of equations,

Mass:
$$\partial_t \overline{\rho} + \nabla \cdot (\overline{\rho} \underline{\widetilde{u}}) = 0$$
 (6.31)

Momentum:
$$\partial_t(\overline{\rho}\underline{\widetilde{u}}) + \nabla \cdot (\overline{\rho}\underline{\widetilde{u}} \otimes \underline{\widetilde{u}}) = -\nabla \overline{p} + \nabla \cdot \underline{\overline{\sigma}} + \nabla \cdot \underline{\sigma}^t$$
 (6.32)

Species:
$$\partial_t(\overline{\rho}\underline{\widetilde{Y}}) + \nabla \cdot (\underline{\rho}\underline{u} \otimes \underline{\widetilde{Y}}) = \nabla \cdot \underline{j} + \nabla \cdot \underline{j}^t + \underline{\widetilde{\omega}}$$
 (6.33)

Total Enthalpy:
$$\partial_t(\overline{\rho}h_t) + \nabla \cdot (\overline{\rho}\underline{\widetilde{u}}h_t) = \nabla \cdot \underline{\overline{q}} + \nabla \cdot \underline{q}^t,$$
 (6.34)

Note that in this case, we do not distinguish between averaging in the RANS-sense (spatial/temporal ensemble) or filtering in the LES sense. Importantly, unclosed terms appear in the Favre-averaged equations. These include:

• Turbulent Stresses:

$$\sigma_{ij}^t = \overline{\rho}\widetilde{u}_i\widetilde{u}_j - \overline{\rho}\widetilde{u_iu_j} = -\overline{\rho}\widetilde{u_i'u_j'}$$
(6.35)

$$=\overline{\rho}\widetilde{u}_{i}\widetilde{u}_{j}-\overline{\rho}[(\widetilde{u}_{i}+u_{i}'')\cdot(\widetilde{u}_{j}+u_{j}'')]$$
(6.36)

$$=\overline{\rho}\widetilde{u}_{i}\widetilde{u}_{j}-\overline{\rho}[\widetilde{\widetilde{u}_{i}}\widetilde{\widetilde{u}_{j}}+\widetilde{\widetilde{u}_{i}}\widetilde{u}_{j}''+\widetilde{u}_{i}''\widetilde{\widetilde{u}_{j}}+\widetilde{u}_{i}''\widetilde{u}_{j}'']$$
(6.37)

where the last two lines contain the expression known as the Leonard Triple Decomposition of the turbulent stresses

• Turbulent Scalar Transport:

$$j_{\alpha,i}^{t} = \overline{\rho}\widetilde{u}_{i}\widetilde{Y}_{\alpha} - \overline{\rho}\widetilde{u_{i}Y_{\alpha}} \cong \overline{\rho}\widetilde{u_{i}'Y_{\alpha}''}$$

$$(6.38)$$

• Turbulent Enthalpy Flux:

$$q_i^t = \overline{\rho}\widetilde{u}_i\widetilde{h}_t = \overline{\rho}\widetilde{u}_i\widetilde{h}_t = \overline{\rho}\widetilde{u}_i'\widetilde{h}_t'' \tag{6.39}$$

• Chemical Source Term:

$$\overline{\omega}_{\alpha} = \sum_{k} W_{\alpha} \nu_{\alpha} k_{f,k} \left[\prod_{\alpha} [Y_{\alpha}]^{\nu'_{\alpha,k}} - \frac{1}{K} \prod_{\alpha} [Y_{\alpha}]^{\nu''_{\alpha,k}} \right]$$
(6.310)

In the following, we pursue a segregated approach and employ different models for each term.

6.4. Closure Models for Turbulent Fluxes and Reynolds Stresses

6.4.1. Turbulent Stresses. A common closure for modeling turbulent stresses is the equilibrium closure approach using the Boussinesq approximation. This relates the turbulent

6. TURBULENT COMBUSTION MODELING

stresses to the shear rate via a turbulent viscosity μ_t ,

$$\overline{\rho u_i'' u_j''} = \overline{\rho} \widetilde{u_i'' u_j''} = -\frac{\mu_t}{\mu} \widetilde{\sigma_{ij}} + \frac{2}{3} \overline{\rho} k \delta_{ij}; \quad k = \frac{1}{2} \widetilde{u_i''^2}, \tag{6.41}$$

$$\widetilde{\sigma}_{ij} = \mu \left[\partial_i \widetilde{u}_j + \partial_j \widetilde{u}_i - \frac{2}{3} \partial_k \widetilde{u}_k \delta_{ij} \right].$$
(6.42)

Within this modeling framework, there exist several closure models for the turbulent viscosity, μ_t . A common closure is the RANS $k - \epsilon$ model, which expresses μ_t as

$$\mu_t = C_\mu \overline{\rho} \frac{k^2}{\epsilon} \tag{6.43}$$

with transport equations for k and ϵ and the model parameter C_{μ} often set equal to a value of $C_{\mu} = 0.09$ to obtain agreement with experimental configurations for isothermal flows.

Another class of closures is based on LES filtering. Specifically, we can write μ_t as,

$$\mu_t = C_s \overline{\rho} \Delta^2 |\hat{S}_{ij}|, \qquad (6.44)$$

$$=\sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}} \tag{6.45}$$

where Δ is the LES filter width and $S_{ij} = (\partial_i \tilde{u}_j + \partial_j \tilde{u}_i)/2$. The constant C_s is referred to as the Smagorinski constant, and generally ranges between values of 0.1 and 0.25. There exists a more sophisticated version of this model, wherein the value of C_s can be dynamically adjusted, due to Germano [25]. Additional models for the turbulent viscosity include nonequilibrium models, fractal methods, and Lagrangian models. It is also important to model the turbulent scalar fluxes of Eq. (6.38) and Eq. (6.39). The most common model for these quantities is based on the eddy-diffusivity concept, relating turbulent scalar fluxes to a resolved (or mean) scalar gradient such that,

$$\overline{\rho u_i''\psi''} = \overline{\rho}\widetilde{u_i''\psi''} = -\overline{\rho}\alpha_t \frac{\partial\overline{\psi}}{\partial x_i}$$
(6.46)

where α_t is the turbulent diffusivity, evaluated as,

$$\alpha_t = C_\psi \Delta^2 |\widetilde{S}_{ij}| \tag{6.47}$$

By introducing the turbulent Schmidt number,

$$Sc_t = \frac{\nu_t}{\alpha_t} \sim [0.4, 0.7] \tag{6.48}$$

and comparing Eq. (6.45) to Eq. (6.47), it follows that,

$$C_{\psi} = \frac{C_s}{Sc_t} \tag{6.49}$$

which is common in the context of LES applications.

6.4.2. Chemical Source Term Modeling. A main focus of turbulent combustion modeling is concerned with the closure of the chemical source term:

$$\overline{\dot{\omega}}_{\alpha} = \overline{\dot{\omega}_{\alpha}(\underline{Y}, T, \rho, ...)} \tag{6.410}$$

From previous flame structure analysis and the Arrhenius form, we know that this term is localized and non-linear, so that a simple approximation of the form,

$$\widetilde{\omega}_{\alpha} \simeq \dot{\omega}_{\alpha}(\underline{\widetilde{Y}}, \overline{\widetilde{T}}, \widetilde{\rho}) \tag{6.411}$$

is inaccurate!

In the following, we will consider a subset of turbulent combustion models that have different fidelity and applicability. In general, we can evaluate turbulent combustion models based on the following properties:

(1) Accuracy

- (2) Generality and Model Applicability
- (3) Computational Complexity

We will now introduce a general classification to categorized different combustion models. For this, we introduce the notion of topology to distinguish between topology-free and topology-based combustion models.

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Topology-Free Models

- Closure models make no assumptions about flame structure, or exploit flame topology
- Combustion model typically requires solution for all or a subset of species (for reduced chemistry)
- Models use different submodels to describe mixing and reaction chemistry

Examples

- Direct source-term evaluation ("laminar chemistry model")
- Eddy-dissipation model/eddybreakup model
- Transported PDF model
- Deconvolution methods

Advantages

- Applicable to wider range of combustion problems
- More general formulation
- Provides representation of different combustion-physical processes: detailed chemistry, complex transport, multistream systems, boundary conditions, heat-transfer, radiation

Disadvantages

- Computationally complex (often due to higher dimensional formulation)
- Segregation of different physical processes (mixing and reaction)
- Statistical convergence (particle method)
- Numerical algorithms

Topology-Based Models

- Closure for chemical source term exploits structure/topology of flame,typically assume presence of a laminar flame element or flamelet
- Flame structure described from asymptotic canonical and laminar flame solutions of premixed and diffusion flames
- Flame structure projected onto a reduced scalar manifold (Z, C, χ) to describe chemistry more compactly

Examples

- steady flamelet model
- flamelet/progress-variable (FPV)
- Flame prolongation of ILDM (intrinsic low dimensional manifold) (FPI)
- Flamelet-generated manifold (FGM)
- Conditional moment closure
- Linear eddy model/1D turbulence

Advantages

- Reduced computational complexity
- Presumed PDF-closure for turbulence-chemistry interaction
- Account for finite-rate chemistry
- Flexibility to incorporate radiation, pollutant formation, unsteady processes, multistream combustion
- Chemistry described via tabulatino

Disadvantages

- Reduced manifold representations eliminate slow-time-scale processes
- Models are specific to certain combustion regimes; other combustion regimes (partially premixed) are only approximately represented
- Dependence on tabulation introduces memory limitations and restrictions on model complexity

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	Premixed	Non-Premixed Diffusion	Partially Premixed
Fast Chemistry	Eddy Dissipation Model (EDM)		
	Reaction ProgressVariable Level Set Bray-Moss-Libby (BML) Model	Mixture Fraction	Reacton Progress Variable + Mixture Fraction
Finite- Rate Chemistry	Laminar finite-rate model (zeroth order source term evaluation) Transported PDF Model Eddy Dissipation Model Linear Eddy Model (LEM)		
	Flame Surface Density Flamelet Formulation (FGM, Level Set) Thickened Flamelet Model	Flamelet Progress Variable Flame Prolongation in ILDM Conditional Moment Closure	

FIGURE 6.41 Classification of combustion models and applications.

6.5. Regime-Independent Models

In the following we will consider different turbulent combustion models. For illustrative purposes, we will consider a simple one-step reaction chemistry of the form,

$$F + O \xrightarrow{k} P.$$
 (6.51)

6.5.1. Laminar Finite Rate Chemistry. We will first consider the transport equations,

$$\rho D_t \widetilde{Y}_{\alpha} = \nabla \cdot (\rho \alpha \nabla \widetilde{Y}_{\alpha}) + \nabla \cdot \underline{j}_{\alpha}^t + \dot{\omega}(\overline{Y}, T, \overline{\rho})$$
(6.52)

The simplest closure model for the chemical source term is then to expand the source term to zeroth order in \underline{Y} and T,

$$\overline{\omega(\underline{Y},T)} \simeq \omega(\underline{\widetilde{Y}},\widetilde{T},\overline{\rho}) \tag{6.53}$$

or,

$$\dot{\omega}_0(\underline{\widetilde{Y}},\widetilde{T}) \simeq \widetilde{Y}_{\rm F}\widetilde{Y}_{\rm O} \exp\left\{-\frac{T_a}{\widetilde{T}}\right\}$$
(6.54)

The fact that this model is not accurate can be seen by expanding to second order:

$$\dot{\omega}(\overline{Y},T) = \widetilde{Y}_{\mathrm{F}}\widetilde{Y}_{\mathrm{O}}\exp\left\{-\frac{T_{A}}{\widetilde{T}}\right\} + \exp\left\{-\frac{T_{A}}{\widetilde{T}}\right\} \left[Y_{\mathrm{F}}''\widetilde{Y}_{\mathrm{O}} + \widetilde{Y}_{F}Y_{\mathrm{O}}'' + \widetilde{Y}_{\mathrm{F}}\widetilde{Y}_{\mathrm{O}}\frac{T_{A}T''}{\widetilde{T}^{2}}\right]$$
(6.55)

6.5.2. Eddy Breakup and Eddy-Dissipation Model. The Eddy Breakup Model (EBU) and Eddy Dissipation Model (EDM) assume that combustion is mixing-controlled, so that finite-rate chemistry effects are neglected. This is computationally inexpensive and useful for mixing-limited combustion, but limited to one- or two-step chemistry. The EBU has been formulated for premixed flames and replaces the chemical timescale by the turbulent mixing timescale $\tau_u = k/\epsilon$,

EBU:
$$\dot{\omega} = \rho C_{EBU} \frac{1}{\tau_u} \sqrt{\overline{Y_P''^2}}$$
 (6.56)

EDM: For
$$D_t \widetilde{Y}_{\alpha} = \nabla \cdot (\rho \alpha \nabla \widetilde{Y}_{\alpha}) + \nabla \cdot \underline{j}_{\alpha} + W_{\alpha} \nu_{\alpha} \overline{w}$$
 (6.57)

and
$$\nu'_{\rm F} \mathbf{F} + \nu'_{\rm O} \mathbf{O} \to \nu_{\rm P} \mathbf{P}$$
 (6.58)

$$w = \rho \frac{1}{\tau_u} \min\left(A \frac{\widetilde{Y}_{\rm F}}{\nu_{\rm F}' W_{\rm F}}, A \frac{\widetilde{Y}_{\rm O}}{\nu_{\rm O}' W_{\rm O}}, A B \frac{\widetilde{Y}_{\rm P}}{\nu_{\rm P}'' W_{\rm P}}\right) \tag{6.59}$$

where $A \approx 4.0$ is an empirical constant. In this case, the chemical reaction is controlled by the large-eddy mixing time τ_u defined in 4.31. The combustion can proceed as soon as turbulence is present, and no ignition source is required to be present. This model is acceptable for premixed flames, but does suffer from issues in predicting ignition and combustion upstream of the flame.

6.5.3. Transported PDF Methods. PDF methods employ a statistical approach for representing turbulent reacting flows. Starting from the work of [52] in the 1980's, these methods have performed reasonably well in describing stochastic aspects of turbulent combustion such as intermittent extinction and re-ignition [53]. An excellent review of the subject can be found in [27]. Instead of solving transport equations for the scalar flow variable, the transport equation for the PDF is solved. The PDF itself is a one-point statistical representation of turbulent reacting quantities, and does not contain information about two/multi-point quantities. In general, we can distinguish between:

- (1) Scalar transported PDF-method: solves a transport equation for the joint scalarenergy PDF $P(\mathcal{Y}, \mathcal{T}; \underline{x}, t)$, where \mathcal{Y}, \mathcal{T} are sample-space variables
- (2) Joint velocity-scalar PDF-method: solves a transport equation for velocity-scalar energy quantities $P(\underline{\mathcal{U}}, \underline{\mathcal{Y}}, \mathcal{T}; \underline{x}, t)$.

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Advantages of PDF methods include:

- Statistical representation of the PDF contains information about all moments of the joint (velocity)-scalar field: $\langle u_i^n Y_{\alpha}^m T^p \rangle(n, m, p) \in \mathbb{Z}$. Note that this information is often more than one needs for engineering representations
- Since the chemical source term is a point-wise quantity, this term is exact and does not require modeling.
- The PDF method does not invoke any assumptions about the flame topology, and is therefore (in theory) a regime-independent method apart from the mixing model

Disadvantages include:

• The resulting transport equation for the joint PDF evolves in state-space and physical space and is therefore higher dimensional:

$$P(\underline{U}, \underline{Y}; \underline{x}, t) \in \mathbb{R}^{(N_D + N_S) \times (N_D + 1)}$$
(6.510)

where:
$$\underline{U} \in \mathbb{R}^{N_D}; \underline{Y} \in \mathbb{R}^{N_S}; \underline{x} \in \mathbb{R}^{N_D}, t \in \mathbb{R}$$
 (6.511)

• Scalar mixing and turbulent transport are governed by multi-dimensional and twopoint interactions. These processes are therefore not fully represented and require modeling. Example: $\epsilon = \overline{\partial_i u_j \partial_j u_i}$

We will now derive the transport equation for the joint velocity-scalar PDF. We can formally write the PDF as

$$P_{\phi}(\psi; \underline{x}, t), \tag{6.512}$$

where $\underline{\phi}(\underline{U}, \underline{Y}, T)^T$ represents a composition or field variable and $\underline{\psi}(\underline{U}, \underline{Y}, T)$ represents a sample space variable. We also recall the definition of the mean quantity or expectation as,

$$\overline{\phi} = \int_{-\infty}^{\infty} \psi P_{\phi}(\psi; \underline{x}, t) d\psi \qquad (6.513a)$$

$$\overline{Q} = \overline{Q}(\underline{x}, t) = \iint_{-\infty}^{\infty} Q(\underline{\psi}) P_{\underline{\phi}}(\underline{\psi}; \underline{x}, t) d\underline{\psi}.$$
(6.513b)

Note that the Favre-PDF \widetilde{P} and the conventional PDF P can be related via the mass density function,

$$\mathcal{P}_{\underline{U},\underline{Y}}(\underline{\mathcal{U}},\mathcal{Y};\underline{x},t) = \overline{\rho}\widetilde{P}_{\underline{U},\underline{Y}}(\underline{U},\underline{Y};\underline{x},t) = \rho P_{\underline{U},\underline{Y}}(\underline{U},\underline{Y};\underline{x},t).$$
(6.514)

A convenient way for deriving the transported PDF method is by introducing the finegrained PDF:

$$\widetilde{P}_{\underline{u},\underline{Y}}(\underline{u},\underline{\mathcal{Y}};\underline{x},t) = \delta(\underline{U}(\underline{x},t) - \mathcal{U})\delta(\underline{Y}(\underline{x},t) - \mathcal{Y}).$$
(6.515)

corresponding to a delta function as representations of the PDF for a single flow-field representation. Details of the derivation of the transported PDF equation can be found in the work of Pope (see Appendix H) [54]. Here, we sketch the derivation and highlight critical evaluation steps. The starting point are the following governing equations:

$$D_t \rho = -\rho \nabla \cdot \underline{u} \tag{6.516}$$

$$D_t \underline{u} = \underline{a}, \quad \underline{a} = \frac{1}{\rho} (-\nabla p + \nabla \cdot \underline{\sigma})$$
 (6.517)

$$D_t \underline{Y} = \underline{b}, \quad \underline{b} = \frac{1}{\rho} (-\nabla \cdot \underline{j} + \underline{\omega})$$
 (6.518)

To illustrate the derivation, we consider an isothermal flow ($\rho = \text{const}$), and then extend this formulation to variable density systems. Thus, in our first analysis we will replace continuity with $\nabla \cdot \underline{u} = 0$. We now consider a scalar, one-point random field variable $Q(\underline{u}, \underline{Y})$ as a function of time. First, the substantial derivative becomes,

$$\overline{D_t Q} = \partial_t \overline{Q} + \nabla \cdot \underline{u} \overline{Q}$$

$$= \partial_t \iint_{-\infty}^{\infty} Q(\underline{\mathcal{U}}, \underline{\mathcal{Y}}) P_{\underline{\mathcal{U}}, \underline{\mathcal{Y}}}(\underline{\mathcal{U}}, \underline{\mathcal{Y}}; \underline{x}, t) d\underline{\mathcal{U}} d\underline{\mathcal{Y}} + \nabla \cdot \left[\iint_{-\infty}^{\infty} \mathcal{U} Q(\underline{\mathcal{U}}, \underline{\mathcal{Y}}) P_{\underline{\mathcal{U}}, \underline{\mathcal{Y}}}(\underline{\mathcal{U}}, \underline{\mathcal{Y}}; \underline{x}, t) d\underline{\mathcal{U}} d\underline{\mathcal{Y}} \right]$$

$$(6.519)$$

$$(6.520)$$

$$= \iint_{-\infty}^{\infty} Q(\underline{U}, \underline{Y}) \left[\partial_t P_{\underline{U}, \underline{Y}} + \nabla \cdot \mathcal{U} P_{\underline{U}, \underline{Y}} \right] d\underline{\mathcal{U}} d\underline{\mathcal{Y}}$$

$$(6.521)$$

Second, we can expand the mean convection term on the LHS of Eq. (6.519) as,

$$D_t Q(\underline{U}, \underline{Y}) = \frac{\partial Q}{\partial \underline{U}} \cdot D_t \underline{U} + \frac{\partial Q}{\partial \underline{Y}} \cdot D_t \underline{Y}$$
(6.522)

$$=\frac{\partial Q}{\partial \underline{U}}\underline{a}+\frac{\partial Q}{\partial \underline{Y}}\underline{b},\tag{6.523}$$

with expected value,

$$\overline{D_t Q} = \overline{\frac{\partial Q}{\partial \underline{U}}}\underline{\underline{a}} + \overline{\frac{\partial Q}{\partial \underline{Y}}}\underline{\underline{b}}.$$
(6.524)

Note that \underline{a} and \underline{b} depend on multi-point information of random field variable \mathcal{U} and \mathcal{Y} , such as the velocity of scalar gradients. Since these multi-point terms are not contained in the formulation, they require modeling; therefore, we represent all unclosed terms in the the vector \underline{C} . With this, we can write,

$$P_{\underline{U},\underline{Y},\underline{C}}(\underline{\mathcal{U}},\underline{\mathcal{Y}},\underline{C}) = P_{\underline{C}|\underline{\mathcal{U}},\mathcal{Y}}(\underline{\mathcal{C}}|\underline{\mathcal{U}},\underline{\mathcal{Y}})P(\underline{\mathcal{U}},\underline{\mathcal{Y}}).$$
(6.525)

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By introducing this step, we can express all right-hand-side terms as,

$$\underline{a} = \underline{a}(\underline{U}, \underline{Y}, \underline{C}) \tag{6.526a}$$

$$\underline{b} = \underline{b}(\underline{U}, \underline{Y}, \underline{C}) \tag{6.526b}$$

$$Q = Q(\underline{U}, \underline{Y}), \tag{6.526c}$$

where \underline{C} describes the two-point closure terms. This allows us to write,

$$\overline{\frac{\partial Q}{\partial \underline{U}}\underline{a}} = \iiint_{-\infty}^{\infty} \frac{\partial Q}{\partial \underline{\mathcal{U}}} (\underline{\mathcal{U}}, \underline{\mathcal{Y}}) \underline{a} (\underline{U}, \underline{Y}, \underline{\mathcal{C}}) P_{\underline{U}, \underline{Y}, \underline{\mathcal{C}}} (\underline{\mathcal{U}}, \underline{\mathcal{Y}}, \underline{C}) d\underline{\mathcal{C}} d\underline{\mathcal{Y}} d\underline{\mathcal{U}}$$
(6.527)

$$= \iint_{-\infty}^{\infty} \frac{\partial Q}{\partial \underline{\mathcal{U}}}(\underline{\mathcal{U}}, \underline{\mathcal{Y}}) \overline{\underline{a} | \underline{\mathcal{U}}, \underline{\mathcal{Y}}} P_{\underline{\mathcal{U}}, \underline{Y}}(\underline{\mathcal{U}}, \underline{\mathcal{Y}}) d\underline{\mathcal{Y}} d\underline{\mathcal{U}}$$
(6.528)

where
$$\underline{a}|\underline{U},\underline{Y} = \int_{-\infty}^{\infty} \underline{a}(\underline{U},\underline{\mathcal{Y}})P_{\underline{C}|\underline{U},\underline{Y}}(\underline{\mathcal{C}}|\underline{\mathcal{U}},\underline{\mathcal{Y}})d\underline{\mathcal{C}}.$$
 (6.529)

Similarly, we have,

$$\overline{\frac{\partial Q}{\partial \underline{U}}}\underline{\overline{b}} = \iint_{-\infty}^{\infty} \frac{\partial Q}{\partial \underline{\mathcal{U}}} (\underline{\mathcal{U}}, \underline{\mathcal{Y}}) \overline{\underline{b}} | \underline{U}, \underline{Y}} P_{\underline{U}, \underline{Y}} (\underline{\mathcal{U}}, \underline{\mathcal{Y}}) d\underline{\mathcal{Y}} d\underline{\mathcal{U}}$$
(6.530)

By using integration-by-parts,

$$\int_{a}^{b} f'gdx = fg\Big|_{a}^{b} - \int_{a}^{b} fg'dx, \qquad (6.531)$$

we can rewrite Eq. (6.528) and Eq. (6.530),

$$\frac{\partial Q}{\partial \underline{U}}a = -\iint_{-\infty}^{\infty} Q \frac{\partial}{\partial \underline{U}} \left[\overline{\underline{a}|\underline{U},\underline{Y}}P_{\underline{U},\underline{Y}}, (\underline{\mathcal{U}},\underline{\mathcal{Y}}) \right] d\underline{\mathcal{Y}}d\underline{\mathcal{U}}$$
(6.532a)

$$\overline{\frac{\partial Q}{\partial \underline{U}}b} = -\iint_{-\infty}^{\infty} Q \frac{\partial}{\partial \underline{Y}} \left[\underline{\underline{b}} | \underline{U}, \underline{Y} P_{\underline{U}, \underline{Y}}, (\underline{\mathcal{U}}, \underline{Y}) \right] d\underline{\mathcal{Y}} d\underline{\mathcal{U}}, \qquad (6.532b)$$

where we have used the fact that the boundary integrals at $\pm \infty$ are zero due to the compact PDF kernel. Upon combining all terms and equating integrands, we obtain the joint velocity-composition PDF transport equation for constant-density flows,

$$\partial_t P_{\underline{U},\underline{Y}} + \underline{\mathcal{U}} \cdot \nabla P_{\underline{U},\underline{Y}} = -\frac{\partial}{\partial \underline{\mathcal{U}}} \left[\overline{\underline{a}|\underline{U},\underline{Y}} P_{\underline{U},\underline{Y}} \right] - \frac{\partial}{\partial \mathcal{Y}} \left[\overline{\underline{b}|\underline{U},\underline{Y}} P_{\underline{U},\underline{Y}} \right], \tag{6.533}$$

where the left-hand terms represent advection in physical space by the unsteady velocity field, the first term on the right-hand side represents transport in velocity space due to conditional acceleration $\overline{\underline{a}|\underline{\mathcal{U}},\underline{\mathcal{Y}}}$, and the last term represents transport in compositional space due to conditional reaction/diffusion $\overline{\underline{b}|\underline{\mathcal{U}},\underline{\mathcal{Y}}}$.
We can at this point make several observations. First, the transport equation evolves in physical-velocity-composition space and cannot be represented by conventional discretization schemes. This is a direct result of the curse of dimensionality. Further, all two-point correlations in $\underline{a}|\underline{U},\underline{\mathcal{Y}}$ and $\underline{b}|\underline{U},\underline{\mathcal{Y}}$ are unclosed and require modeling; this includes such phenomena as molecular diffusion, turbulent mixing, viscous dissipation, and pressure fluctuations. The one-point chemical source term, however, appears in closed form:

$$\overline{\underline{a}|\underline{\mathcal{U}},\underline{\mathcal{Y}}} = \overline{\frac{1}{\rho}(\nabla \cdot \underline{\sigma} - \nabla p)|\underline{\mathcal{U}},\underline{\mathcal{Y}}}$$
(6.534)

$$\overline{\underline{b}|\underline{\mathcal{U}},\underline{\mathcal{Y}}} = \frac{1}{\rho}(-\nabla j)|\underline{\mathcal{U}},\underline{\mathcal{Y}}| + \frac{\omega}{\rho}(\underline{\mathcal{Y}}).$$
(6.535)

In the following, we will consider the joint compositional PDF. We fill first derive this quantity before stating the density-weighted/Favre-weighted PDF and discussing the closure model in the limit of high Reynolds-number flows. Finally, we will discuss solution methods utilizing particle-based approaches.

The joint composition PDF is obtained by integrating over velocity space, resulting in a marginal PDF. The transport equation for this PDF can be written as,

$$\partial_t(\overline{\rho}\widetilde{P}_{\underline{Y}}) + \nabla \cdot (\overline{\rho}\underline{\widetilde{u}}\widetilde{P}_{\underline{Y}}) = -\overline{\rho}\frac{\partial \underline{\dot{\omega}}\widetilde{P}_{\underline{Y}}}{\partial \underline{Y}} - \nabla \cdot (\overline{\underline{u}''|\underline{Y}}\overline{\rho}\widetilde{P}_{\underline{Y}}) + \frac{\partial}{\partial \mathcal{Y}}\left[\frac{1}{\rho}\nabla \cdot \underline{j}|\underline{Y}\overline{\rho}\widetilde{P}_{\underline{Y}}\right], \quad (6.536)$$

where the remaining unclosed terms are the scalar-conditional velocity fluctuation (penultimate right hand term) and the scalar molecular mixing (last right-hand term).

Modeling of conditional diffusion and molecular transport $\underline{b}|\underline{\mathcal{U}},\underline{\mathcal{Y}}$ is of main concern in the PDF closure. Although significant progress has been made, its closure is the weakest link. This term represents transport of the PDF by molecular diffusion. Relevant processes include both transport in physical space and transport in composition space. Molecular transport is typically negligible for high Reynolds number flows at $Sc \sim 1$ and $Pr \sim 1$. By expanding the diffusion term (for constant density and diffusivity), we can see that only the conditional diffusion portion of the molecular mixing term requires modeling:

$$\overline{\alpha\nabla^{2}\underline{Y}|\underline{\mathcal{U}},\underline{\mathcal{Y}}} = \alpha\nabla^{2}\overline{\underline{Y}} + \overline{\alpha\nabla^{2}\underline{Y}'|\underline{\mathcal{U}},\underline{\mathcal{Y}}},$$
(6.537)

where only the last right hand term remains unclosed. Closure models for conditional diffusion should fulfill the following constraints and requirements:

- (1) Scalar mean must remain unchanged
- (2) Correct representation of joint scalar dissipation rate
- (3) Velocity and scalar gradients must remain uncorrelated
- (4) Local scalar isotropy must be correct
- (5) PDF of conserved scalar should relax to Gaussian distribution
- (6) All scalars must remain bounded

- (7) Mixing should be local in composition space
- (8) Mixing rate should depend on scalar length scale
- (9) Mixing should depend on Re, Sc, Da, etc.

By considering the unclosed term:

$$\overline{\alpha \nabla^2 Y' | \underline{\mathcal{U}}, \underline{\mathcal{Y}}} \tag{6.538}$$

describing molecular mixing, we can justify the following requirements for a conserved scalar representation:

- (1) Gaussianity: follows from the law of large numbers
- (2) Molecular mixing must leave scalar mean unchanged. Specifically, integrating molecular mixing over the PDF $P_{U,Y}$ should give

$$\iint \overline{\alpha \nabla^2 Y' | \underline{\mathcal{U}}, \underline{\mathcal{Y}}} P_{\underline{\mathcal{U}}, \underline{Y}} d\underline{\mathcal{U}} d\underline{\mathcal{Y}} = \overline{\alpha \nabla^2 \underline{Y'}^2} = 0$$
(6.539)

for constant α

(3) The representation of the joint scalar dissipation rate can be written as follows,

$$\iint Y_{\alpha}' \overline{\alpha \nabla^2 Y_{\beta}' | \underline{\mathcal{U}}, \underline{\mathcal{Y}}} P_{\underline{\mathcal{U}}, \underline{Y}} d\underline{\mathcal{U}} d\mathcal{Y}_{\alpha} d\mathcal{Y}_{\beta} = \alpha \overline{(Y_{\alpha}' \nabla^2 Y_{\beta}')}$$
(6.540)

$$= \alpha \nabla \cdot (Y'_{\alpha} \nabla Y'_{\beta}) - \alpha \nabla Y'_{\alpha} \cdot \nabla Y'_{\beta}$$
(6.541)

(4) The locality of mixing in composition space should be represented such that molecular diffusion in physical space is local and continuous in both space and time. For instance, with $\chi_{\alpha} = 2\alpha_{\alpha} (\nabla Y_{\alpha})^2$,

$$dY_{\alpha} = \sqrt{\frac{\chi_{\alpha}}{2\alpha_{\alpha}}} dx \tag{6.542}$$

with χ_{α} continuous. We can then expect that dY_{α} remains continuous in composition space.

6.5.3.1. Interaction by Exchange with the Mean (IEM). We will now give an overview of some important mixing models. The first of these is known as Interaction by Exchange with the Mean (IEM). This is one of the simplest models, in which we assume a linear relaxation of the scalar \mathcal{Y}_{α} towards its mean \overline{Y}_{α} . The model formulation is thus,

$$\overline{\alpha \nabla^2 Y_{\alpha}' | \underline{\mathcal{U}}, \underline{\mathcal{Y}}} - \frac{1}{\tau_{\alpha}} \overline{\underline{Y}} - \underline{\mathcal{Y}}), \qquad (6.543)$$

where τ_{α} is the mixing time scale, which is here related to the scalar dissipation rate of species α ,

$$\tau_{\alpha} = \frac{\overline{Y_{\alpha}^{\prime 2}}}{\chi_{\alpha}} \quad \chi_{\alpha} = 2\alpha_{\alpha} \overline{(\nabla Y_{\alpha}^{\prime})^2} \tag{6.544}$$



FIGURE 6.51 Coalesce-Disperse model schematic.

The closure for τ_{α} is obtained through scale similarity:

$$\tau_u = \frac{k}{\epsilon}; \quad \tau_\alpha = \frac{Y_\alpha'^2}{\chi_\alpha} \quad C_\alpha = \frac{\tau_u}{\tau_\alpha}, \tag{6.545}$$

where a value of $C_{\alpha} \approx 2$ is commonly used. This mixing model of Eq. (6.543) fulfills the following conditions,

- Does not change the mean value
- Correct representation of the joint scalar dissipation
- Independence of the velocity and scalar gradients requires,

$$\overline{\alpha_{\alpha}\nabla Y_{\alpha}'|\underline{\mathcal{Y}}} = \frac{1}{\tau_{\alpha}}(\overline{Y_{\alpha}|\underline{\mathcal{U}}} - \mathcal{Y}_{\alpha})$$
(6.546)

• Linearity

The main issues with this model are that the PDF does not relax to a Gaussian distribution and that the mixing is not local.

6.5.3.2. *Coalesce-Disperse Model.* A second well-known mixing model is the Coalesce-Disperse (CD) model due to Curl [17] describes the mixing as a two-step process of a dispersed two-fluid system as in Fig. 6.51.

In such a model, fluid 1 with $(Y_{\alpha,1}, Y_{\beta,1})$ interacts with fluid 2, characterized by $(Y_{\alpha,2}, Y_{\beta,2})$. After interaction, the fluids are characterized by $(Y_{\alpha,1}^*, Y_{\beta,1}^*)$ and $(Y_{\alpha,2}^*, Y_{\beta,2}^*)$. This means that in the mixed state,

$$Y_{\alpha}^{*} = \frac{1}{2}(Y_{\alpha,1} + Y_{\alpha,2}) \tag{6.547}$$

$$Y_{\beta}^{*} = \frac{1}{2}(Y_{\beta,2} + Y_{\beta,2}). \tag{6.548}$$

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Properties of this model include that the mean remains unchanged and that mixing occurs at a characteristic frequency. Disadvantages include lack of Gaussianity, equal mixing time for all scalars, and the fact that mixing is not local. This last issue is particularly true for the limit of $Da \to \infty$, in which the flame sheet becomes infinitely small.

6.5.3.3. Numerical Methods. A last aspect of the PDF methods that we will discuss is the Lagrangian PDF method and the Fokker-Planck equation. The transported PDF equation was originally derived in Eulerian form, and requires solution in joint space-time-(velocity)-composition space. This is computationally expensive, and becomes infeasible for problems involving even a moderate number of chemical species. To overcome this issue, we can formulate the PDF equation as an equivalent particle method using stochastic differential equations. The first method for accomplishing this task combines the Langevin model for the velocity field with the species equations such that,

$$d\underline{x}^{+} = [\underline{\overline{u}} + \nabla \alpha_T]^{+} dt + \sqrt{(2\alpha_T)^{+}} dW, \qquad (6.549)$$

where \underline{u} is obtained from RANS/LES and dW is an independent Wiener process with zero mean and unit variance such that,

$$dW(t) = W(t + dt) - W(t) \equiv \mathcal{N}(0, dt).$$
(6.550)

The first term on the right-hand side of Eq. (6.549) describes drift while the second term describes the difference resultant from stochastic evolution of the physical process. The species evolution is then evaluated as,

$$\frac{d\underline{Y}^{+}}{dt} = \underline{\omega}(\underline{Y}^{+}(t)) + (\alpha \nabla^{2} \underline{Y})^{+}, \qquad (6.551)$$

where the first right hand term is a pointwise exact source term while the second term on the RHS is an unclosed two-point species diffusion. By modeling the molecular mixing term using the IEM model of Eq. (6.543) we can obtain the following Lagrangian particle model,

$$d\underline{X}^{+} = [\underline{\overline{u}} + \nabla \alpha_{T}] dt + \sqrt{2\alpha_{T}} d\underline{W}$$
(6.552)

$$d\underline{\phi}^{+} = \underline{\omega}(\underline{\phi}^{+}(t)) - \frac{1}{\tau_{M}}(\underline{\phi}^{+} - \overline{\phi}^{+})$$
(6.553)

$$\underline{\phi} = (\underline{Y}, T), \tag{6.554}$$

where τ_M is the turbulent mixing rate. The second method for approaching this type of model deals with the case of homogeneous turbulence. In this situation, we can omit the momentum conservation and only consider a stochastic differential equation for species conservation

$$d\phi = \underline{\omega}dt - \underline{a}dt + \underline{b}dW,\tag{6.555}$$

where the term $\underline{\omega}dt$ represents reaction chemistry, the term $\underline{a}dt$ represents drift by molecular mixing, and the term $\underline{b}dW$ represents diffusion. In this case, we can write \underline{a} and \underline{b} as,

$$\underline{a} = \frac{1}{\tau_M} (\underline{\phi} - \overline{\phi}) \tag{6.556}$$

$$\underline{b} = \frac{1}{\tau_M} (\overline{\underline{\phi'}^2} f(\underline{\phi})), \qquad (6.557)$$

where $f(\phi)$ is introduced to enforce boundedness in composition space.

6.5.4. Linear Eddy Model (LDM). Another class of turbulent combustion model, the Linear Eddy Model, was developed as a subgrid model for LES and is generally considered regime-independent. The key idea behind this model is that we can represent the flame structure as a collection of one-dimensional flame elements. The turbulence-chemistry interaction is represented by a triple-map, which is followed by reaction and diffusion.



FIGURE 6.52 Subgrid representation of LDM.

For each 1D flame element, we can solve a 1D reaction-diffusion equation:

$$\rho \frac{\partial Y_{\alpha}}{\partial t} = \frac{\partial}{\partial \xi} j_{\alpha} + \dot{\omega}_{\alpha} \tag{6.558}$$

$$\rho c_p \frac{\partial T}{\partial t} = \rho \sum_{\alpha=1}^{N_s} c_{p,\alpha} j_\alpha \frac{\partial T}{\partial \xi} + \frac{\partial}{\partial \xi} \left(\lambda \frac{\partial}{\partial \xi} T \right) + \dot{\omega}_T, \qquad (6.559)$$

where ξ is a local coordinate. By introducing $\underline{\phi} = (\underline{Y}, T)$, turbulence-chemistry interaction is then represented through a triple-map,

$$\underline{\phi}(\xi) \to \underline{\phi}(M(\xi)) \tag{6.560}$$

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where,

$$M(\xi) = \begin{cases} 3\xi & 0 \le \xi \le l/3\\ 2l - 3\xi & l/3 \le \xi \le 2l/3\\ 3\xi - 2l & 2l/3 \le \xi \le l\\ \xi & \text{else} \end{cases}$$
(6.561)

Advection of 1D flame elements is incorporated through *splicing* to accommodate mass conservation and element coupling.

6.5.5. One Dimensional Turbulence. This type of modeling represents an extension of the IEM multiscale approach to couple reaction, diffusion, and turbulent transport. It combines a coupled deterministic solution for reaction and molecular transport with a stochastic prescription for turbulent transport. Lagrangian formulations and Eulerian representations are both solved. More details on this model can be found in [37].

Discussion Box 15: Turbulent Compositional Fluctuations in RCMs.

The modeling of low-Mach turbulence is important in practical combustion devices, and this is particularly easy to observe within the context of Rapid Compression Machines (RCMs) [31]. Within an RCM, gas is ignited via rapid piston compression. Such devices are often used to study aspects of reaction kinetics and form a better understanding of fuel mixtures such as syngas. While a major goal of RCMs is to provide a homogeneous, repeatable environment in which to study combustion phenomena, the generation of turbulence within these machines can cause discrepancies between experimental measurements and the results of simulation or theory. Several mechanisms by which this can occur are as follows:

- (1) *Filling process*: The filling process of the driven section with the fresh test gas mixture is accompanied by the generation of small-scale turbulence fluctuations that are approximately homogeneously distributed in the entire test section. If the compression phase is initiated directly after the filling process, providing insufficient time for the complete decay, the initially introduced turbulence is amplified during the compression
- (2) Corner vortices: During the compression phase, the piston motion generates corner vortices and large vortical structures. The roll-up of these structures induces flow field perturbations and the entrainment of cold fluid into the core region. Although these corner vortices can be reduced by appropriate piston-crown design, their contributions cannot be entirely eliminated.
- (3) Boundary layer-generated turbulence: During the compression phase, the piston motion induces a mean flow, which leads to the formation of a boundary layer. At sufficiently high Reynolds numbers, the boundary layer transitions, which is associated with the generation of turbulence. This wall-generated turbulence is subsequently transported into the core region, where it will be further amplified through the mean strain interaction.
- (4) Turbulence production by compressive strain: During the compression phase, the rapid piston motion induces a time-dependent strain rate, leading to enhanced turbulence production. This nonequilibrium process is dependent on the strain-rate profile, and is a main mechanism for the turbulence amplification at the end of the compression phase.

Amongst the key conclusions from this study were that turbulence-chemistry interaction could cause stochastic ignition characteristics, and that fluctuations in temperature and composition are important reasons for systematic errors in RCM measurements, which are critical for understanding chemistry.

6.6. Topology-Based Combustion Models

The key idea behind topology based combustion models is that we can utilize information about the underlying flame topology to (a) obtain a closure of unclosed/model terms and (b) reduce the dimensional complexity of the model. Since these models rely on the underlying flame topology, they tend to be grouped into the asymptotic limits of premixed flame models and diffusion flame models. Of course, regime dependence can restrict applicability and accuracy of the combustion model if not applied carefully and appropriately. Often, these models are referred to as either flamelet models or tabulated chemistry models. The concept of a flamelet was introduced in Discussion Box 11. A flamelet is a representation of a flame as an ensemble of laminar diffusion/premixed flames – the fundamental assumption in this case is that turbulent structures do not penetrate the flame, and thus only lead to deformation and stretching of the reaction-diffusion region. In analyzing these types of schemes, we will start by revisiting the flamelet model for diffusion flames.

6.6.1. Flamelet Models. In the derivation of the flamelet equations, the following assumptions are introduced:

- (1) Typically derived for low-Mach number flows
- (2) Derivation in the limit of large *Da* flows requires an assumption that chemical time scales are fast compared to turbulent flow scales, and it is difficult ot incorporate the effects of slow time scales (NO formation, radiation, soot, etc.)
- (3) Flamelet derivation depends on solution of a boundary-value problem with welldefined conditions in the fuel/oxidizer streams; extensions to multi-stream systems is therefore difficult

For the formal model derivation of the flamelet equation, we consider the scalar equation,

$$\rho \partial_t \phi + \rho \underline{u} \cdot \nabla \phi = \rho \alpha \nabla^2 \phi + \rho \underline{\dot{\omega}} \tag{6.61}$$

$$\rho \partial_t Z + \rho \underline{u} \cdot \nabla Z = \rho \alpha \nabla^2 Z, \tag{6.62}$$

where we have assumed equal diffusivity, Le = 1, and constant transport properties. Now, consider a surface of stoichiometric mixture, and construct the local coordinate system as shown in Fig. 6.61 (this is equivalent to a Crocco-transform). Formally, we can evaluate



FIGURE 6.61 Coordinate system for flamelet equation derivation.

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directions as,

$$\underline{\hat{n}} = \frac{\nabla Z}{|\nabla Z|}; \quad \underline{\hat{s}} = \frac{\hat{n} \times \hat{e}}{|\hat{n} \times \hat{e}|}, \quad t = -\underline{\hat{n}} \times \underline{\hat{s}}; \quad d\underline{x} = \underline{\hat{n}} \frac{dZ}{|\nabla Z|}, \tag{6.63}$$

so that $\underline{\hat{n}}$ is aligned with the mixture-fraction gradient. We now introduce a coordinate transformation:

$$(t,\underline{x}) \to (\tau, Z(\underline{x}, t), Z_2, Z_3)$$
 (6.64)

and transformation rules,

$$\frac{\partial}{\partial t} = \frac{\partial \tau}{\partial t} \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t} \partial Z \tag{6.65}$$

$$\nabla = \nabla Z \frac{\partial}{\partial Z} + \nabla_{\perp}; \quad \nabla_{\perp} = \left(0; \frac{\partial}{\partial Z_2}; \frac{\partial}{\partial Z_3}\right)^T.$$
(6.66)

Applying the transformation rule to the governing equations gives:

$$\rho \frac{\partial \underline{\phi}}{dt} - \frac{1}{2} \rho \chi_Z \frac{\partial^2 \underline{\phi}}{\partial Z^2} - \rho \underline{\dot{\omega}} = -\rho \underline{u} \cdot \nabla_\perp \phi + \rho_\alpha \nabla_\perp^2 \phi + 2\rho_\alpha \nabla Z \cdot \nabla_\perp \phi, \qquad (6.67)$$

where $\underline{\phi} = (\underline{y}, H)^T$ and $\underline{\dot{\omega}} = (\underline{\underline{\omega}}^T, q_R)^T$. An asymptotic analysis with stretched coordinates,

$$\xi = \frac{1}{\epsilon} (Z - Z_{st}) \tag{6.68}$$

with $\epsilon \sim 1/E_A$ gives the following,

$$\rho \frac{\partial \phi}{\partial t} - \frac{1}{2} \rho \chi_Z \frac{\partial^2 \phi}{\partial Z^2} = \rho \underline{\omega}$$
(6.69)

$$\chi_Z = \chi_{Z,\text{st}} \exp\left\{2\left([\text{erfc}^{-1}(2Z_{\text{st}})]^2 - [\text{erfc}^{-1}(2Z)]^2\right)\right\}.$$
(6.610)

By invoking the steady state assumption, we can precompute all flamelet solutions for different χ_{st} and parameterize all thermochemical quantities in terms of Z and χ_{st} ,

$$\psi = \mathcal{E}_{\psi}(Z, \chi_{\rm st}) \tag{6.611}$$

with:
$$\psi = (\nu, \alpha, \underline{\dot{\omega}}, T, \underline{Y})^T$$
. (6.612)

Closure of the averaged conservation equations for low Mach number flows gives:

$$\partial_t \overline{\rho} + \nabla \cdot (\overline{\rho} \underline{\widetilde{u}}) = 0 \tag{6.613}$$

$$\overline{\rho}\partial_t \underline{\widetilde{u}} + \overline{\rho}\underline{\widetilde{u}} \cdot \nabla \underline{\widetilde{u}} = -\nabla \overline{p} + \nabla \cdot \underline{\overline{g}} + \nabla \cdot \underline{\underline{\tau}}^*$$
(6.614)

$$\underline{\overline{\sigma}} = \overline{\mu} [\nabla \underline{\widetilde{u}} + (\nabla \underline{\widetilde{u}})^T] - \frac{2}{3} \overline{\mu} \nabla \underline{\widetilde{u}} \underline{I}.$$
(6.615)

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where τ^* represents contributions from other sources to the momentum equation. Filtered quantities and other quantities are then obtained using a presumed PDF closure model:

$$\underline{\widetilde{\psi}} = \iint \mathcal{E}_{\psi}(Z, \chi_Z) \widetilde{P}(Z, \chi_Z) dZ d\chi_Z, \qquad (6.616)$$

where $\tilde{P}(Z, \chi_Z)$ is the joint PDF of Z and χ_Z . A common model for $\tilde{P}(Z, \chi_Z)$ is obtained by writing,

$$\widetilde{P}(Z,\chi_Z) = \frac{\rho}{\overline{\rho}} P(Z,\chi_Z) = \frac{\rho}{\overline{\rho}} P(Z) P(\chi_Z)$$
(6.617)

under the assumption of statistical independence, and we use,

$$P(Z) = \beta(Z, \widetilde{Z}, \widetilde{Z''^2}) \tag{6.618}$$

by writing $\chi_Z = \chi_{Z,\text{st}} f(Z)$ so that we only need to model $P(\chi_{\text{st}})$. A common model is to represent $P(\chi_{\text{st}})$ with a log-normal distribution ($\chi_{\text{st}} \ge 0$),

$$P(\chi_{\rm st}) = \frac{1}{\chi_{\rm st}\sigma\sqrt{2\pi}} \exp\left\{-\frac{(\ln\chi_{\rm st}-\mu)^2}{2\sigma^2}\right\}$$
(6.619)

with $\sigma \approx 1$ and $\mu = \ln \overline{\chi_{st}}$. Note that the model requires transport equations for $\widetilde{Z}, \widetilde{Z''^2}$ and an algebraic model for χ_{st} .

Note that there are several modifications to this formulation. These can include:

- Flamelet/Progress-Variable (FPV) Model
- Flamelet-Generated Manifold (FGM)
- Flame Prolongation of ILDM

In the last two models, the flamelet state space is commonly constructed from premixed flamelet solutions.

6.6.2. Flamelet Model for Turbulent Diffusion Flames. The formulation and derivation of the flamelet model for turbulent diffusion flames presented here follows that due to Peters [48]. The Steady Laminar Flamelet Model (SLFM) describes turbulent flames from the solution of the steady laminar flamelet equations by including the upper stable branch and mixing branch of the S-curve.

The Flamelet Progress Variable (FPV) Model represents a parameterization of the state-space of Eq. (6.611) using the mixture fraction and the progress variable [32, 49],

$$\psi = g_{\psi}(Z, C). \tag{6.620}$$

As shown in Fig. 6.62a and Fig. 6.62b, the FPV model represents relaxation to a steady S-curve in state space while the SLFM represents projection onto a steady S-curve.



FIGURE 6.62 Steady laminar flamelet model (a) corresponds to vertical projection onto the S-curve in state-space, while FPV model (b) relaxes to a steady S-curve.

6.7. Turbulent Premixed Combustion Models

To use flamelet models for premixed combustion, we introduce a progress variable C that is defined by the normalized temperature,

$$C = \frac{T - T_u}{T_b - T_u}.$$
 (6.71)

In the limit that the flame is infinitely thin, we can represent the distribution of C as,

$$P(C) = \beta\delta(C) + (1 - \beta)\delta(1 - C).$$

$$(6.72)$$

The transport equation for the \widetilde{C} follows then as,

$$\overline{\rho}\partial_t \widetilde{C} + \overline{\rho} \widetilde{\underline{u}} \cdot \nabla \widetilde{C} = \nabla \cdot (\overline{\rho} \overline{\alpha} \nabla \widetilde{C}) + \nabla \cdot (\overline{\rho} \overline{u'' C''}) + \overline{\dot{m}}_C.$$
(6.73)

A conventional model for the source term is,

$$\overline{\dot{m}}_C = \overline{\rho}_u s_L I_0 \Sigma \tag{6.74}$$

with ρ_u the density in the unburned mixture, s_L the laminar burning velocity, I_0 the stretch, Σ flame surface density (flame surface per unit volume). Algebraic model for Σ ,

$$\Sigma \sim \frac{\tilde{C}(1-\tilde{C})}{\tilde{L}_y},\tag{6.75}$$

with \widetilde{L}_y the crossing length scale. The transport equation for Σ can be obtained,

$$\partial_t \Sigma + \nabla \cdot (\underline{\widetilde{u}}\Sigma) = \nabla \cdot (\rho \alpha_t \nabla \Sigma) + C_1 \frac{\epsilon}{k} \Sigma - C_2 s_L \frac{\Sigma^2}{1 - \overline{C}}$$
(6.76)



FIGURE 6.71 Definition of the progress variable.

Other models include the Coherent Flame Model – however, this model does not contain any information about chemistry.

6.7.1. Level Set Equation for Premixed Flames. We now introduce a distance function $G(\underline{x}, t)$ that defines distance to the flame. Note that we take $G(\underline{x}_F, t) = G_0$. The conservation equation for G can be written as,

$$D_t G = 0. (6.77)$$

From the kinematic balance at the flame front, we have,

$$\frac{dx}{dt} = \underline{u} + s_L \cdot \underline{\hat{n}}; \quad \underline{\hat{n}} = -\frac{\nabla G}{|\nabla G|}, \tag{6.78}$$

upon rearranging, we have,

$$D_t G = s_L |\nabla G|, \tag{6.79}$$

which is a purely kinematic equation. Note that the influence of chemistry is introduced through s_L , and that s_L depends on strain, curvature, Lewis number, and other hydrodynamic and mixture parameters.



FIGURE 6.72 Definition of the level-set variable G.

At this point, we proceed to analysis of the regime diagram for turbulent combustion. As shown in Fig. 6.73, there exist several key combustion regimes:

- Laminar flame: Re < 1
- Wrinkled flame: $u' < s_L$: In this case, the turn-over velocity u' of the largest eddies is not large enough to compete with the advancement of eddies of the flame front at the laminar burning velocity. This regime is not relevant for practical applications.
- Broken reaction zone: only present in the limit of high u'/s_L
- Corrugated flamelet regime: u' > Sc, Re > 1, $Ka_{\delta} < 1$, with $Ka = \tau_{\rm F}/t_{\eta} \rightarrow l_{\rm F} < \eta$. In this regime, the entire reactive-diffusive structure of length scale $l_{\rm F}$ is embedded within eddies of size η . The flame is not perturbed by turbulent fluctuations and remains quasi-steady. Note that if $l_{\rm F} \sim \eta$, the flame will transition from the corrugated regime to the thin reaction zone regime. The $l_{\rm F} = \eta$ equivalency is known as the Klimov-Williams condition.
- Thin Reaction Zone Regime: Re > 1, $Ka_{\delta} < 1$, Ka < 1. The fact that Ka < 1 implies that the smallest eddies of size η can enter into the reactive-diffusive flame structure since $\eta < l_{\rm F}$. The smallest eddies, however, are still larger than the inner layer thickness $l_{\rm F}$ such that $\eta < l_{\delta} \equiv l_{\rm F}$. In this case, there is no penetration into

6.7. TURBULENT PREMIXED COMBUSTION MODELS



FIGURE 6.73 Regime diagram for turbulent combustion.

the inner layer, and only broadening of the flame structure occurs as a result of turbulence.

Given these different combustion regimes, it is now useful to consider several different models for premixed turbulent flames. The first of these is the G-Equation, which is defined as



FIGURE 6.74 Schematic of the corrugated flamelet regime.



FIGURE 6.75 Schematic of the thin reaction zone regime.

follows,

$$D_t G = s_L |\nabla G|. \tag{6.710}$$

The burning velocity model,

$$s_L = s_L^0 - s_L^0 \mathcal{M}\kappa - \mathcal{M}s, \qquad (6.711)$$

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where the second right hand term is the curvature and the third right hand term is the strain. The curvature is defined as,

$$\kappa = \nabla \cdot \underline{\hat{n}} = \nabla \cdot \left(-\frac{\nabla G}{|\nabla G|} \right), \tag{6.712}$$

the strain is,

$$s = -\underline{\hat{n}} \cdot \nabla \underline{u} \cdot \underline{\hat{n}} \tag{6.713}$$

and the Markstein length \mathcal{M} defines the effects of heat-release on flame location. To solve this level set equation, we define G as a field variable using a signed distance function $|\nabla G| = 1$. We can then solve the advection equation for G with a closure model for the flame speed being dependent on the combustion regime.

Consider, for instance, the thin reaction zone regime. The temperature field evolves as,

$$\rho D_t T = \nabla \cdot (\rho \alpha \nabla T) + \rho \dot{\omega}_T. \tag{6.714}$$

meaning that the propagation of the isosurface $T(\underline{x}, t) = T_0$ is governed by,

$$\partial_t T + \nabla T \cdot \left. \frac{dx}{dt} \right|_{T=T_0} = 0 \tag{6.715}$$

and its motion is defined as,

$$\left. \frac{dx}{dt} \right|_{T=T_0} = u_0 + \underline{\hat{n}} s_d \tag{6.716}$$

where the displacement speed is defined as,

$$s_d = \left| \frac{\nabla \cdot (\rho \alpha \nabla T) + \rho \dot{\omega}_T}{\rho |\nabla T|} \right|_{T_0}, \tag{6.717}$$

and

$$\underline{\hat{n}} = -\frac{\nabla T}{|\nabla T|}\Big|_{T=T_0}.$$
(6.718)

In this case, the G-Equation closure is,

$$D_t G = \left[\frac{\nabla \cdot (\rho \alpha \nabla T) + \rho \dot{\omega}_T}{\rho |\nabla T|}\right] |\nabla G|$$
(6.719)

By splitting the displacement speed into normal and tangential components, we obtain,

$$\nabla \cdot (\rho \alpha \nabla T) = -\rho \alpha |\nabla T| \nabla \cdot \underline{\hat{n}} + \underline{\hat{n}} \cdot \nabla (\rho \alpha \underline{\hat{n}} \cdot \nabla T)$$
(6.720)

which gives,

$$D_t G = (s_n + s_r) |\nabla G| - \alpha \kappa |\nabla G| \tag{6.721}$$

By normalizing the G-Equation with the Kolmogorov scaling,

$$t^* = \frac{t}{t_{\eta}}; \quad x^* = \frac{x}{\eta}; \quad \underline{u}^* = \frac{u}{u_{\eta}};$$
 (6.722)

$$\kappa^* = \kappa \eta; \quad \nabla^* = \eta \nabla \tag{6.723}$$

we obtain the following with $s_{L,s} = s_n + s_r$,

$$\partial_{t^*}G + \underline{u}^* \cdot \nabla^*G = \frac{s_{L,s}}{u\eta} |\nabla^*G| - \frac{\alpha}{\nu} \kappa^* |\nabla^*G|$$
(6.724)

For the thin reaction zone regime $s_{L,s} < u_{\eta}$, and for the corrugated regime $s_L^0 > u_{\eta}$. Thus, the leading order model equation for both regimes becomes,

$$\rho \partial_t G + \rho \underline{u} \cdot \nabla G = (\rho s_L^0) \sigma - (\rho \alpha) \kappa \sigma; \quad \sigma = |\nabla G| \tag{6.725}$$

The closure for RANS/LES is obtained by presumed PDF-Model:

$$\overline{\sigma}(\underline{x},t) = \int_{-\infty}^{\infty} GP(G,\underline{x},t)dG$$
(6.726)

$$\overline{G'^2}(\underline{x},t) = \int_{-\infty}^{\infty} [G - \overline{G}]^2 P(G,\underline{x},t) dG, \qquad (6.727)$$

which gives,

$$\rho \partial_t \widetilde{G} + \overline{\rho} \widetilde{\underline{u}} \cdot \nabla \widetilde{G} + \nabla \cdot (\overline{\rho} \overline{u'' G''}) = (\rho s_L^0) \overline{\sigma} - (\rho \alpha) \overline{\kappa} \overline{\sigma}$$
(6.728)

CHAPTER 7

Selected Topics

CHAPTER 8

Example Cantera Code

8.1. Demo Cantera Notebook

```
ME471DemoNotebook
                              June 7, 2017
In [1]: from __future__ import print_function
       import cantera as ct
       import cantera
       import numpy as np
       import matplotlib.pylab as plt
       import sys, os
       import pandas as pd
       %matplotlib inline
In [84]: def compute_flame_speed_and_sensitivities(gs):
            # Simulation parameters
            width = 0.03 \# m
            initial_grid = [0.0,0.001,0.01,0.015,0.02,0.029,0.03]
            # Flame object
            f = ct.FreeFlame(gs)
            f.set_refine_criteria(ratio=2, slope=0.1, curve=0.14)
            f.solve(loglevel=1, refine_grid=True ,auto=True)
            # Use the adjoint method to calculate sensitivities
            sens = f.get_flame_speed_reaction_sensitivities()
            return f, sens
        def print_sensitivities(gs, sns):
            print('Rxn # k/S*dS/dk Reaction Equation')
            print('-----
                                                            -----')
            for m in range(gs.n_reactions):
                print('{: 5d} {: 10.3e} {}'.format(
                     m, sns[m], gs.reaction_equation(m)))
        def print_flame_speed(sl):
            flsp = sl.u[0]
            print('Flame speed: %f ' % (flsp))
            return flsp
                                  1
```

```
def print_gas_params(gs):
            TPX = qs.TPX
            gs.equilibrate('HP', solver='gibbs')
            t_ad = gs.T
            cp_ad = gs.cp_mass
            gs.TPX = TPX
            phi = (gs.mole_fraction_dict()['CH4']/gs.mole_fraction_dict()['O2'])/
            print('CH4 mole fraction: %f' % gs.mole_fraction_dict()['CH4'])
            print('02 mole fraction: %f' % gs.mole_fraction_dict()['02'])
            print('N2 mole fraction: %f' % gs.mole_fraction_dict()['N2'])
            print('Equivalence ratio: %f' % phi)
            print('Unburned specific heat capacity: %f' % gs.cp_mass)
            print('Burned specific heat capacity: %f' % cp_ad)
            print('Adiabatic flame temperature: %f' % t_ad)
        def get_x_vec(ky,fs):
            return fs.X[fs.gas.species_index(ky)]
        def get_y_vec(ky,fs):
            return fs.Y[fs.gas.species_index(ky)]
        def get_mw(ky,fs):
            return fs.gas.molecular_weights[fs.species_index(ky)]
        def print_sensitivities(gs):
            print()
            print('Rxn # k/S*dS/dk
                                       Reaction Equation')
            print('-----
                                                               -----')
            for m in range(gs.n_reactions):
                print('{: 5d} {: 10.3e} {}'.format(
                      m, sens[m], qs.reaction_equation(m)))
        def norm_vec(vc):
            return [v/max(vc) for v in vc ]
In [72]: #Computing flame speed
        p = ct.one_atm # pressure [Pa]
        Tin = 300.0 # unburned gas temperature [K]
        mech = '/home/jdunnmon/Research/Mechanisms/gri30/grimech30.cti'
        gas_obj = ct.Solution(mech, 'gas')
        reactants = 'CH4:0.5, 02:1, N2:3.76'
        gas_obj.transport_model = 'Mix'
        gas_obj.TPX = Tin, p, reactants
        print_gas_params(gas_obj)
CH4 mole fraction: 0.095057
02 mole fraction: 0.190114
                                   2
```

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```
N2 mole fraction: 0.714829
Equivalence ratio: 1.000000
Unburned specific heat capacity: 1077.338911
Burned specific heat capacity: 1514.344414
Adiabatic flame temperature: 2225.524583
In [73]: sol, sens = compute_flame_speed_and_sensitivities(gas_obj)
********** Solving on 6 point grid with energy equation enabled ***********
. . .
Attempt Newton solution of steady-state problem...
                                               failure.
                                4.337
Take 10 timesteps 2.136e-05
Attempt Newton solution of steady-state problem...
                                               failure.
Take 10 timesteps 0.0005474
                               2.871
Attempt Newton solution of steady-state problem...
                                               failure.
Take 10 timesteps 0.002338
                               3.919
Attempt Newton solution of steady-state problem...
                                                failure.
Take 10 timesteps
                 5.852e-05
                               5.895
Attempt Newton solution of steady-state problem...
                                                failure.
Take 10 timesteps 2.083e-05
                              6.13
Attempt Newton solution of steady-state problem...
                                                failure.
Take 10 timesteps 0.0003559
                               4.887
Attempt Newton solution of steady-state problem...
                                                failure.
Take 10 timesteps 0.009121 3.422
Attempt Newton solution of steady-state problem...
                                                failure.
Take 10 timesteps 0.1558
                              2.308
Attempt Newton solution of steady-state problem... success.
Problem solved on [7] point grid(s).
. . .
grid refinement disabled.
In [74]: print('Flame speed = %f' % (sol.u[0]))
Flame speed = 0.379667
In [83]: zz = sol.flame.grid-0.03
        #Plotting
        plt.figure(figsize=[6,4])
        plt.plot(zz, sol.T/1000, 'k-', label='T/1000')
```

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