We are discussing gaseous combustion in a mixture of perfect gases containing \( N \) species indexed with \( k=1 \) to \( N \):

\[
p = \sum_{k=1}^{N} p_k \quad \text{where} \quad p_k = \rho_k \frac{R}{W_k} T
\]

\[
\rho = \sum_{k=1}^{N} \rho_k
\]

\[
p = \rho \frac{R}{W} T
\]
### STOICHIOMETRY AND EQUVALENCE RATIO:

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Definition</th>
<th>Useful relations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass fraction $Y_k$</td>
<td>Mass of species $k$ / Total Mass</td>
<td>$Y_k$</td>
</tr>
<tr>
<td>Mole fraction $X_k$</td>
<td>Moles of species $k$ / Total moles</td>
<td>$X_k = \frac{W}{W_k} Y_k$</td>
</tr>
<tr>
<td>Molar concentration $[X_k]$</td>
<td>Moles of species $k$ / Unit volume</td>
<td>$[X_k] = \rho \frac{Y_k}{W_k} = \rho \frac{X_k}{W}$</td>
</tr>
<tr>
<td>Mean molecular weight $W$</td>
<td>$\frac{1}{W} = \sum_{k=1}^{N} \frac{Y_k}{W_k}$ and $W = \sum_{k=1}^{N} X_k W_k$</td>
<td></td>
</tr>
</tbody>
</table>

\[
\nu'_F F + \nu'_O O \rightarrow Products
\]

\[
\left( \frac{Y_O}{Y_F} \right)_{st} = \frac{\nu'_O W_O}{\nu'_F W_F} = s
\]

Stoichiometric ratio

\[
\phi = s \frac{Y_F}{Y_O} = \left( \frac{Y_F}{Y_O} \right) / \left( \frac{Y_F}{Y_O} \right)_{st}
\]

Equivalence ratio
FUEL / AIR COMBUSTION COMPOSITION
AT EQUIVALENCE RATIO $\phi$

$$Y_F = \frac{1}{1 + (1 + 3.76W_{N_2}/W_{O_2}) s/\phi}$$

<table>
<thead>
<tr>
<th>Global reaction</th>
<th>$s$</th>
<th>$Y_{F}^{st}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CH_4 + 2(O_2 + 3.76N_2)$ $\rightarrow CO_2 + 2H_2O + 7.52N_2$</td>
<td>4.00</td>
<td>0.055</td>
</tr>
<tr>
<td>$C_3H_8 + 5(O_2 + 3.76N_2)$ $\rightarrow 3CO_2 + 4H_2O + 18.8N_2$</td>
<td>3.63</td>
<td>0.060</td>
</tr>
<tr>
<td>$2C_8H_{18} + 25(O_2 + 3.76N_2)$ $\rightarrow 16CO_2 + 18H_2O + 94N_2$</td>
<td>3.51</td>
<td>0.062</td>
</tr>
<tr>
<td>$2H_2 + (O_2 + 3.76N_2)$ $\rightarrow 2H_2O + 3.76N_2$</td>
<td>8.00</td>
<td>0.028</td>
</tr>
</tbody>
</table>

With air, combustible mixtures contain typically more than 90 % of... air! This will be useful for theory: a combustible mixture will essentially have the same properties (density, viscosity, conductivity) as pure air.

In a combustion code:

- In a non reacting compressible flow (aerodynamics), we have 5 variables:
  - 3 velocities
  - pressure or temperature or enthalpy or entropy
  - density

- In combustion, we have 5 + (N-1) unknown 3D fields to determine:
  - 3 velocities
  - pressure or temperature or enthalpy or entropy
  - N species -> actually N-1 since their sum is unity
  - density

- We need 5 + (N-1) equations:
  - Momentum (3)
  - Energy, or enthalpy or entropy or temperature
  - Continuity for each species (or for N-1 species + total mass)
Continuity equations (N):

\[ \frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho (u_i + V_{k,i}) Y_k \right) = \omega_k \quad \text{for } k = 1 \text{ to } N \]

Summing them from 1 to N MUST give the continuity equation:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \]

So that we need:

\[ \sum_{k=1}^{N} Y_k V_{k,i} = 0 \quad \sum_{k=1}^{N} \omega_k = 0 \]

Diffusion velocities: careful...

(Williams 1985 or Ern and Giovangigli 1994)

- The \( V_k \)'s are obtained by solving this system:

\[ \nabla X_p = \sum_{k=1}^{N} \frac{X_p X_k}{D_{pk}} (V_k - V_p) + (Y_p - X_p) \frac{\nabla p}{P} + \frac{p}{p} \sum_{k=1}^{N} Y_p Y_k (f_p - f_k) \quad \text{for } p = 1, N \]

- This is the diffusion matrix which must be inverted at each point at each instant... but almost no one does it.

We use simplified forms

\[ V_k = -D_k \frac{\nabla X_k}{X_k} \]

- FICK's law
- HIRSCHFELDER's law
What are the $D_k$'s?

- The diffusion coefficients of species $k$ in the MIXTURE
- Not the binary diffusion coefficients $D_{ij}$ of kinetic gas theory
- Obtained by:
  \[ D_k = \frac{1 - Y_k}{\sum_{j \neq k} X_j / D_{jk}} \]
- All $D_k$'s are different in general...
- $D_k$'s vary significantly but their ratios to thermal diffusivity $D_{th}$ vary much less. They are measured by the Lewis number of each species:
  \[ Le_k = \frac{\lambda}{\rho C_p D_k} = \frac{D_{th}}{D_k} \]

Lewis numbers are not intrinsic parameters of a species. They depend on the mixture

Lewis numbers of main species in a stoechiometric CH4/air premixed flame
The need for correction velocities if Lewis numbers are different:

\[ L_{e_k} = \frac{\lambda}{\rho C_p D_k} = \frac{D_{th}}{D_k} \]

The \( D_k \)'s are not equal if \( Le_k \) differ

\[ \frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} (\rho (u_i + V_{k,i}) Y_k) = \dot{\omega}_k \]

\[ V_k = -D_k \frac{\nabla X_k}{X_k} \]

Summing the species equations with Fick's law:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho \sum_{k=1}^{N} D_k \frac{W_k}{W} \frac{\partial X_k}{\partial x_i} \right) \]

which is not zero if all Lewis numbers are not equal.

A correction velocity \( V_{c} \) is required:

\[ \frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} (\rho (u_i + V_{k,i}) Y_k) = \dot{\omega}_k \]

Replace:

\[ V_k = -D_k \frac{\nabla X_k}{X_k} \]

By:

\[ V_k = -D_k \frac{\nabla X_k}{X_k} + V_c \]

Adding all species equations gives:
\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho \sum_{k=1}^{N} D_k \frac{W_k}{W} \frac{\partial X_k}{\partial x_i} - \rho V_i^c \right)
\]

\(V_i^c\) can be chosen to ensure mass conservation:

\[
V_i^c = \sum_{k=1}^{N} D_k \frac{W_k}{W} \frac{\partial X_k}{\partial x_i}
\]

and the proper expression of the diffusion velocity is:

\[
V_k = -D_k \frac{\nabla X_k}{X_k} + V_c = -D_k \frac{\nabla X_k}{X_k} + \frac{1}{W} \sum_{k=1}^{N} D_k W_k \nabla X_k
\]

Conclusion: careful of codes using simplified expressions for diffusion velocities with non-equal Lewis numbers.

**Momentum equations (3)**

\[
\frac{\partial}{\partial t} \rho u_j + \frac{\partial}{\partial x_i} \rho u_i u_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} + \rho \sum_{k=1}^{N} Y_k f_{k,j} = \frac{\partial \sigma_{ij}}{\partial x_i}
\]

Same form in non-reacting flows. Except that:
- density here has very strong gradients
- viscosity changes rapidly with temperature

\[
\tau_{ij} = -\frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]
Last but not least: energy

- Each code uses a different form for energy, enthalpy or temperature
- All forms of course are equivalent (should be...)
- The trick is not to confuse them and beware of simplified forms...
- Compressible vs incompressible is one source of confusion
- Total versus other forms of energy is another one
- Full summary in PV2011 Chapter 1

<table>
<thead>
<tr>
<th>Form</th>
<th>Energy</th>
<th>Enthalpy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensible</td>
<td>( e_s = \int_{T_0}^{T} C_v dT - RT_0/W )</td>
<td>( h_s = \int_{T_0}^{T} C_p dT )</td>
</tr>
<tr>
<td>Sensible + Chemical</td>
<td>( e = e_s + \sum_{k=1}^{N} \Delta h_{f,k} Y_k )</td>
<td>( h = h_s + \sum_{k=1}^{N} \Delta h_{f,k} Y_k )</td>
</tr>
<tr>
<td>Total Chemical</td>
<td>( e_t = e + \frac{1}{2} u_i u_i )</td>
<td>( h_t = h + \frac{1}{2} u_i u_i )</td>
</tr>
<tr>
<td>Total non Chemical</td>
<td>( E = e_s + \frac{1}{2} u_i u_i )</td>
<td>( H = h_s + \frac{1}{2} u_i u_i )</td>
</tr>
</tbody>
</table>

\[
C_p = \sum_{k=1}^{N} C_{pk} Y_k = \sum_{k=1}^{N} C_{pk}^m \frac{Y_k}{W_k}
\]

\( C_p \) depends both on temperature (through the \( C_{pk}'s \)) and on the composition (the \( Y_k's \)
Molar heat capacity of each species change with temperature

- Good starting point: total energy $e_t$

\[
\frac{\partial \rho e_t}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i e_t) = -\frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_j} (\sigma_{ij} u_i)
\]

$\sigma_{ij} = \tau_{ij} - p\delta_{ij}$

careful with the heat flux. It is not:

\[
q_i = -\lambda \frac{\partial T}{\partial x_i}
\]

but is also includes the flux transported by species diffusion:

\[
q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{k=1}^{N} h_k Y_k V_{k,i}
\]
The heat release and the reaction rates of species

- There are \( N \) reaction rates \( \dot{\omega}_k \) in the species equations (one for each species)

- But only one heat release term:

\[
\dot{\omega}_T = - \sum_{k=1}^{N} \dot{\omega}_k \Delta H_f^0
\]
Many authors also like to work with the temperature equation.

If pressure is constant:

\[
\rho C_p \frac{DT}{Dt} = \dot{\omega}_T' + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) - \rho \frac{\partial T}{\partial x_i} \left( \sum_{k=1}^{N} C_{p,k} Y_k V_{k,i} \right)
\]

Careful with this new ‘heat release’

---

Two reaction rate terms: same name in the literature but NOT equal

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i E) = \dot{\omega}_T + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) + \frac{\partial}{\partial x_j} (\sigma_{ij} u_i)
\]

\[
\dot{\omega}_T = - \sum_{k=1}^{N} \dot{\omega}_k \Delta H^0_{f_k}
\]

\[
\rho C_p \frac{DT}{Dt} = \dot{\omega}_T' + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) - \rho \frac{\partial T}{\partial x_i} \left( \sum_{k=1}^{N} C_{p,k} Y_k V_{k,i} \right)
\]

\[
\dot{\omega}_T' = - \sum_{k=1}^{N} h_k \dot{\omega}_k = - \sum_{k=1}^{N} h_{s_k} \dot{\omega}_k - \sum_{k=1}^{N} \Delta H^0_{f_k} \dot{\omega}_k
\]
\[
\omega'_T = - \sum_{k=1}^{N} h_k \dot{\omega}_k = - \sum_{k=1}^{N} h_{sk} \dot{\omega}_k - \sum_{k=1}^{N} \Delta H^0_{jk} \dot{\omega}_k = - \sum_{k=1}^{N} h_{sk} \dot{\omega}_k + \dot{\omega}_T
\]

**If the \( C_{p,k} \) s are equal:** \( C_{p,k} = C_p \)

\[
h_{sk} = \int C_{p,k} dT = \int C_p dT = h_k
\]

so that

\[
\sum_{k=1}^{N} h_{sk} \dot{\omega}_k = h_k \sum_{k=1}^{N} \dot{\omega}_k = 0
\]

\[
\dot{\omega}_T = \dot{\omega}'_T
\]

And if the \( C_{p,k} \) s are equal: \( C_{p,k} = C_p \)

\[
\sum_{k=1}^{N} C_{p,k} Y_k V_{k,i} = C_p \sum_{k=1}^{N} Y_k V_{k,i} = 0
\]

so that the temperature equation:

\[
\rho C_p \frac{dT}{Dt} = \dot{\omega}'_T + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) - \rho \frac{\partial T}{\partial x_i} \left( \sum_{k=1}^{N} C_{p,k} Y_k V_{k,i} \right)
\]

becomes:

\[
\rho C_p \frac{dT}{Dt} = \dot{\omega}'_T + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right)
\]
SUMMARY:

- We have the basic equations
- We can solve them numerically for real flames
- Before we do that, we anticipate that we are going to have difficulties with:
  - Kinetics
  - Turbulence
  - Very large domains
- We are going to need models. Better: we are going to need understanding...otherwise the work is impossible
- To do this we need to study a few academic (canonical) cases even if it means simplifying things a little bit.

So... canonical cases are needed to understand the basic flame features:

- The premixed laminar flame
  - Ch. 2
- The laminar diffusion flame
  - Ch. 3
PREMIXED LAMINAR FLAME

- Under certain assumptions, an explicit resolution of the previous equations is possible
- This is the case for the premixed laminar flame

A one-dimensional steady problem in the reference frame of the flame

\[
\rho u = \text{constant} = \rho_1 s_L
\]

\[
\frac{\partial}{\partial x} \left( \rho (u + V_k) Y_k \right) = \dot{\omega}_k
\]

\[
\rho C_p u \frac{\partial T}{\partial x} = \dot{\omega}_T' + \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) - \frac{\partial T}{\partial x} \left( \rho \sum_{k=1}^{N} C_{p,k} Y_k V_k \right)
\]

No momentum equation needed: we need it only to find pressure changes
This equation can be solved for a large number of species numerically
(CHEMKIN, COSILAB, CANTERA, FLAME MASTER)
But doing so does not tell us much. Let us keep simplifying.

Additional assumptions

- Single reaction limited by fuel (lean). Instead of N mass fractions, we can track one only: \( Y_f \). We assume that \( Y_0 = c_t \)
- All Lewis numbers equal to unity

\[
\rho u = \text{constant} = \rho_1 u_1 = \rho_1 s_L
\]

\[
\rho_1 s_L \frac{dY_F}{dx} = \frac{dx}{dx} \left( \rho D \frac{dY_F}{dx} \right) + \dot{\omega}_F
\]

\[
\rho_1 C_p s_L \frac{dT}{dx} = \frac{dx}{dx} \left( \lambda \frac{dT}{dx} \right) - Q \dot{\omega}_F
\]

- Can solve this by hand! \(-> \) famous field for mathematicians/combustion experts (Williams, Linan, Matalon)
**Simplest solutions**

- If Lewis = 1 temperature and fuel mass fractions are directly linked if properly scaled:

\[ Y = \frac{Y_F}{Y^1_F} \quad \text{and} \quad \Theta = \frac{C_p(T - T_1)}{QY^1_F} = \frac{T - T_1}{T_2 - T_1} \]

- Then:

\[ \theta + Y = 1 \]

- We are left with only one variable to solve for: the reduced temperature (also called the progress variable)

**Master equation for laminar premixed flames:**

\[ \rho_{1sL} \frac{d\Theta}{dx} = \frac{d}{dx} \left( \frac{\lambda}{C_p} \frac{d\Theta}{dx} \right) - B_1 (T_1 + \Theta(T_2 - T_1))^\beta \rho(1-\Theta) \exp \left( -\frac{T_{a1}}{T_1 + \Theta(T_2 - T_1)} \right) \]

\[ \tilde{\omega}_T \]

This is where asymptotics enter the field. Not the topic of present lectures.

Let us summarize the results.
In this simplified world, a flame is:

- dominated by a strongly non linear reaction rate:
  \[ \dot{\omega}_T \]

- decomposed in two zones: a preheating region and a reaction zone

\[ (1-\alpha)/\beta \exp(-1-\beta/\alpha) \]

\[ \text{Reduced temperature } \theta = (T-T_1)/(T_2-T_1) \]
has a thickness given by

\[ \delta = \frac{\lambda_1}{\rho_1 C_p S_L} = \frac{D_{th}^1}{S_L} \]

Heat diffusivity in the fresh gas

or

\[ \frac{\delta S_L}{D_{th}^1} = 1 \]

The Reynolds number of the flame is unity:

\[ \text{Re}_{\text{flame}} = \frac{\delta S_L^0}{\nu} = 1 \]

has a flame speed which depends on the form assumed for reaction rate and molecular diffusion:

<table>
<thead>
<tr>
<th>Model</th>
<th>Fuel reaction rate ( \dot{\omega}_F ) in Eq. (2.22)</th>
<th>Transport assumptions</th>
<th>Flame speed ( s_L )</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZFK</td>
<td>( B_1 T^\beta \rho Y_F e^{-T_s/T} )</td>
<td>( \lambda = \lambda_1 (T/T_1)^{1-\beta_1} ) ( \frac{1}{\beta} e^{-\frac{F_1}{\beta}} (2</td>
<td>B_1</td>
</tr>
<tr>
<td>Williams</td>
<td>( B_1 T^\beta \rho Y_F e^{-T_s/T} )</td>
<td>( \lambda = \lambda_1 (T/T_1)^{1-\beta_1} ) ( \frac{1}{\beta} e^{-\frac{F_1}{\beta}} (2</td>
<td>B_1</td>
</tr>
<tr>
<td>Van Kalmthout</td>
<td>( B_1 \rho Y_F Y_O e^{-T_s/T} )</td>
<td>( \lambda = \lambda_1 T/T_1 ) ( \frac{1}{\beta} e^{-\frac{F_1}{\beta}} (2</td>
<td>B_1</td>
</tr>
<tr>
<td>Echekki</td>
<td>( \rho R_e (1 - \Theta) \theta (\Theta - \Theta_c) )</td>
<td>( \lambda = \lambda_1 T/T_1 ) ( \left( \frac{1}{\beta (\beta - 1)} D_{th}^1 R_e \right)^{1/2} )</td>
<td></td>
</tr>
<tr>
<td>This book</td>
<td>( \rho R_e (1 - \Theta) \theta (\Theta - \Theta_c) )</td>
<td>( \lambda = \lambda_1 ) ( \left( \frac{1}{\beta (\beta - 1)} D_{th}^1 R_e \right)^{1/2} )</td>
<td></td>
</tr>
</tbody>
</table>

You can find the results in TNC 2011 and the derivations in asymptotic papers but let us focus on an important result:
In all premixed flame speed expressions:

\[ s_L \propto \left( \frac{1}{D_{th}} R_r \right)^{1/2} \]

- Multiply the kinetics constant by 4: it will increase the flame speed by two
- Without diffusivity... no premixed flame
- Flame propagation is the combination of both diffusion and reaction

**Flame propagation:**

\[ T(t_0) \]

\[ T(t_1) \]

**DIFFUSION**

**COMBUSTION**
A useful feature of premixed flames:

\[ S_L \propto (D_{th}^1 R_t)^{1/2} \]

Heat diffusivity \hspace{1cm} Kinetics constant

Divide the kinetics constant by a factor \( F > 1 \) and multiply the diffusivity by \( F \). You will get the same flame speed.

But the thickness will be larger by a factor \( F \):

\[ \delta = \frac{D_{th}^1}{S_L} \hspace{1cm} \delta = \frac{FD_{th}^1}{S_L} \]

A useful property in codes: thicken the flame (O’Rourke and Bracco JCP 1979+ CERFACS 90s)

\[ \frac{d}{dt}(\rho Y_k) = \frac{\partial}{\partial x_i} (\rho D \frac{\partial Y_k}{\partial x_i}) + A \rho Y_1 Y_2 ... Y_n \exp\left(-\frac{T_a}{T}\right) \]

\[ \frac{d}{dt}(\rho Y_k) = \frac{\partial}{\partial x_i} (\rho F D \frac{\partial Y_k}{\partial x_i}) + A \frac{\rho Y_1 Y_2 ... Y_n \exp\left(-\frac{T_a}{T}\right)}{F} \]

Same flame speeds with both equations!
In a numerical world where we fight with resolution... this can help!

Thickened and unthickened flames for CH4/air. F=20

For heat release: it is much easier when the flame is thick...
The other case where theory can be developed and is heavily used. Most approaches rely on passive scalars and on the mixture fraction $z$.

**WHAT IS A PASSIVE SCALAR?**

- A scalar quantity which does NOT have a source term (i.e., not a chemical species or a temperature)

$$
\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_i Z}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Z}{\partial x_i} \right)
$$

Ch. 2 Sec 3.2.1
A USEFUL PROPERTY OF PASSIVE SCALARS:

- IF TWO PASSIVE SCALARS $Z_1$ and $Z_2$ HAVE THE SAME BOUNDARY CONDITIONS:
  - IF THEY ARE EQUAL AT $t=0$, THEY WILL ALWAYS REMAIN EQUAL
  - IF THEY DIFFER AT $t=0$, THEY WILL CONVERGE TO THE SAME VALUE AFTER A FEW CHARACTERISTIC TIMES

- DEMO: by considering the norm of $(Z_2-Z_1)$ OR by intuition

INTUITIVE DEMO:

\[
\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_i Z}{\partial x_i} = \frac{\partial}{\partial x_i} (\rho D \frac{\partial Z}{\partial x_i})
\]

can also be written:

\[
\rho \frac{D Z}{D t} = \frac{\partial}{\partial x_i} (\rho D \frac{\partial z}{\partial x_i})
\]

where $D/Dt$ is the total derivative (the variations along the trajectories)
Consider two passive scalars $Z_1$ and $Z_2$. Along trajectories $Z = Z_2 - Z_1$ changes only because of diffusion

$$\frac{DZ}{Dt} = \frac{\partial}{\partial x_i} (\rho D \frac{\partial z}{\partial x_i})$$

- with boundary condition: $Z = 0$
- If the initial condition is $Z = 0$, all gradients are zero and $Z$ will remain 0
- If the initial condition is not $Z = 0$, any non-zero fluid element will go to $Z = 0$ rapidly.

WHAT IS MIXTURE FRACTION?

- A PASSIVE SCALAR WHICH GOES FROM 1 IN THE FUEL TO 0 IN OXIDIZER STREAM

\[
\frac{\partial \rho z}{\partial t} + \frac{\partial \rho u_i z}{\partial x_i} = \frac{\partial}{\partial x_i} (\rho D \frac{\partial z}{\partial x_i})
\]

$z = 1$  
Stream 1: Temperature $T_p^0$  
Fuel mass fraction $Y_p^0$

$z = 0$  
Stream 2: Temperature $T_o^0$  
Oxidizer mass fraction $Y_o^0$

ANY PASSIVE SCALAR GOING FROM 1 IN THE FUEL TO 0 IN THE OXIDIZER IS EQUAL TO THE MIXTURE FRACTION
WHAT DOES IT TAKE TO BE ABLE TO CONSTRUCT A MIXTURE FRACTION?

- H1: Constant pressure and equal Cp’s
- H2: All Lewis numbers equal to unity
- H3: Global single step reaction

\[ \nu_F F + \nu_O O \rightleftharpoons \nu_P P \]

\[ \omega_O = s \hat{\omega}_F \quad s = \frac{\nu_O W_O}{\nu_F W_F} \]

\[ \frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_k) = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_k}{\partial x_i} \right) + \hat{\omega}_k \]

So that we can track only \( T, Y_F \) and \( Y_O \)

IN THE ABSENCE OF COMBUSTION: PURE MIXING

\[ \frac{\partial \rho Y_F}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_F) = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_F}{\partial x_i} \right) \]

\[ \frac{\partial \rho Y_O}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_O) = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_O}{\partial x_i} \right) \]

\[ \frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i T) = \frac{\partial}{\partial x_i} \left( \frac{\lambda}{C_p} \frac{\partial T}{\partial x_i} \right) \]

THREE PASSIVE SCALARs WITH THE SAME EQUATION. IF WE CAN NORMALIZE THEM TO HAVE THE SAME BOUNDARY CONDITIONS, THEY ARE EQUAL TO \( z \)
NORMALIZE THE PASSIVE SCALARS:

\[
\frac{\partial \rho Y_F}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_F) = \frac{\partial}{\partial x_i} \left( \frac{\rho D}{\partial x_i} \right)\left( \frac{\partial Y_F}{\partial x_i} \right) / Y_F^0
\]

\[
\frac{\partial \rho Y_O}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_O) = \frac{\partial}{\partial x_i} \left( \frac{\rho D}{\partial x_i} \right)\left( \frac{\partial Y_O}{\partial x_i} \right) / Y_O^0
\]

\[
\frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i T) = \frac{\partial}{\partial x_i} \left( \frac{\lambda}{C_p} \right)\left( \frac{\partial T}{\partial x_i} \right) / (T_F^0 - T_O^0)
\]

THREE SCALED PASSIVE SCALARS:

\[
Z_1 = Y_F / Y_F^0
\]

\[
Z_2 = 1 - Y_O / Y_O^0
\]

\[
Z_3 = (T - T_O^0) / (T_F^0 - T_O^0)
\]

<table>
<thead>
<tr>
<th></th>
<th>FUEL</th>
<th>OXI</th>
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</thead>
<tbody>
<tr>
<td>(Z_1)</td>
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<td>0</td>
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<tr>
<td>(Z_2)</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>(Z_3)</td>
<td>1</td>
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</tbody>
</table>

THREE PASSIVE SCALARS WITH THE SAME EQUATION AND SAME BC: THEY ARE EQUAL. WE CALL THEM THE MIXTURE FRACTION \(z\)

\[
Z_1 = Z_2 = Z_3 = z
\]
\[ Y_F = Y_F^0 z \quad \text{and} \quad Y_O = Y_O^0 (1 - z) \]

\[ T(z) = z T_F^0 + (1 - z) T_O^0 \]

**The Mixing Lines (No Combustion)**

**Interpretation of z: A Mass Weighted Measurement of Mixing**

- At a given point in the chamber:
  - mass coming from stream 1 = \( m_1 \)
  - mass of fuel = \( m_1 Y_F^0 \)
  - mass coming from stream 2 = \( m_2 \)
  - total mass = \( m_1 + m_2 \)
  - fuel mass fraction \( Y_F = \frac{m_1 Y_F^0}{m_1 + m_2} \)
  - mixture fraction \[ z = \frac{Y_F}{Y_F^0} = \frac{m_1}{m_1 + m_2} \]
INTERPRETATION OF $z$:

If the mixture fraction at this point at time $t$ is $z$, it means that at this point, in 1 kg of mixture:
- $z$ kg come from stream 1
- $(1-z)$ kg come from stream 2

Careful: this works only if all Lewis numbers are equal

With combustion, $z$ can also be introduced:

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

$$
\frac{\partial \rho Y_O}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_O) = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_O}{\partial x_i} \right) + s \dot{\omega}_F
$$

$$
\frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i T) = \frac{\partial}{\partial x_i} \left( \frac{\lambda}{C_p} \frac{\partial T}{\partial x_i} \right) - \frac{Q}{C_p} \dot{\omega}_F
$$

Combining them two by two to eliminate source terms and normalizing to have the same boundary conditions leads to three passive scalars with identical bcs: they are all equal to the mixture fraction $z$
The mixture fraction $z$:

$$z = \frac{sY_F - Y_O + Y_O^0}{sY_F^0 + Y_O^0} = \frac{C_p}{Q}(T - T_O^0) + Y_F^0 = \frac{C_p}{Q}(T - T_O^0) + Y_F - Y_O^0$$

In these expressions, only $Y_F$, $Y_F$ and $T$ are variable.

All other quantities are fixed:
- $s$ is the stoichiometric ratio
- $Y_F^0$ and $Y_O^0$ are the fuel and oxidizer inlet mass fractions in stream 1 and 2 respectively
- $Q$ is the heat of reaction per unit mass

Another property of the mixture fraction $z$: it does not change in a reacting zone

State 1: $Y_F^1, Y_O^1$

$$z_1 = \frac{sY_F^1 - Y_O^1 + Y_O^0}{sY_F^0 + Y_O^0}$$

State 2: $Y_F^1 - \Delta Y_F^1, Y_O^1 - s\Delta Y_F^1$

$$z_2 = \frac{s(Y_F^1 - \Delta Y_F^1) - (Y_O^1 - s\Delta Y_F^1) + Y_O^0}{sY_F^0 + Y_O^0} = z_1$$
How can we use the mixture fraction $z$?

$$z = \frac{sY_F - Y_O + Y^0_O}{sY_F^0 + Y_O^0} \quad = \frac{C_p(T - T^0_O) + Y_F}{sC_p(Q) (T^0_F - T^0_O) + Y_F^0} \quad = \frac{sC_p(T - T^0_O) + Y_O - Y^0_O}{sC_p(Q)(T^0_F - T^0_O) - Y^0_O}$$

Nice to have a quantity without source term

But not sufficient. We can compute $z$ in multiple flows but from $z$ we cannot obtain $T$, $Y_F$ and $Y_O$: in the above expressions, we have relations for couples of variables but not for individual variables.

We need additional assumptions: the simplest one is the infinitely fast assumption

---

**The infinitely fast chemistry assumption**

- Suppose that kinetics are *faster* than all flow processes: fuel and oxidizer cannot co-exist. There will be a ‘fuel’ side ($Y_F=0$) and an oxidizer side ($Y_O=0$)

$$z = \frac{sY_F - Y_O + Y^0_O}{sY_F^0 + Y_O^0} \quad = \frac{C_p(T - T^0_O) + Y_F}{sC_p(Q)(T^0_F - T^0_O) + Y_F^0} \quad = \frac{sC_p(T - T^0_O) + Y_O - Y^0_O}{sC_p(Q)(T^0_F - T^0_O) - Y^0_O}$$

- That is enough to close the problem. For example, on the fuel side:

  $$Y_F(z) = \frac{zY_F^0 + (z - 1)Y^0_O}{s} = Y_F^0 \frac{z - z_{st}}{1 - z_{st}}$$

  $$Y_O(z) = 0.$$

  $$T(z) = zT_F^0 + (1 - z)T_O^0 + \frac{QY_F^0}{C_p} \frac{z_{st} 1 - z}{1 - z_{st}}$$
The z diagram with infinitely fast chemistry and unity Lewis numbers

There are multiple other z diagrams of growing complexity

Ch. 3, Sect 3.5
OK we have $T, Y_k = f(z)$. So what?

- What we really want is to have $T$ and all $Y_k$’s as functions of time and spatial positions. Does $z$ help us?

- Yes: the introduction of $z$ represents a significant simplification as described now:

Instead of solving:

\[
\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_k) = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_k}{\partial x_i} \right) + \dot{\omega}_k
\]

\[
\rho C_p \frac{DT}{Dt} = \dot{\omega}_T + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) - \rho \frac{\partial T}{\partial x_i} \left( \sum_{k=1}^{N} C_{p,k} Y_k V_{k,i} \right)
\]

Only solve the $z$ equation:

\[
\frac{\partial \rho z}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i z) = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial z}{\partial x_i} \right)
\]

And read $T$ and $Y_k$ in the $z$ diagram. We'll use this in turbulent flames.
Think of the $z$ diagram as trajectories:

**MIXING PHASE:** First you mix and reach a given $z$...

**Combustion phase:** after mixing, you burn. And you stop burning when you reach the equilibrium lines.
Possible states: cant be outside the triangle limited by equilibrium and mixing lines

\[ \phi = sY_F/Y_O \]

Parenthesis - a useful tool for codes:

- In 3D codes, one often needs to know the local equivalence ratio
  \[ \phi = sY_F/Y_O \]

- Since \( Y_F \) and \( Y_O \) change because of combustion, the above expression cannot be used to know the local equivalence ratio except in the unburnt gases

- Mixing lines allow to do this: wherever you are in a reacting flow, if you know \( z \), you can find the local equivalence ratio

\[ Y_F = Y_F^0 z \quad \text{and} \quad Y_O = Y_O^0 (1 - z) \]

\[ \phi = \frac{sY_F^0}{Y_O^0} \frac{z}{(1 - z)} \]

**ONLY IF LEWIS = 1**
Example:

- Through a premixed flame front, \( z \) does not change but the local equivalence ratio does change from the fresh gas equivalence ratio to 0 in the burnt gas (for lean flames)

\[
\phi = \frac{sY_F}{Y_O}
\]

- Since \( z \) does not change through the flame front, we can compute the equivalence ratio of the mixture before combustion (on the mixing line) with:

\[
\phi = \frac{sY_F^0}{Y_O^0} \frac{z}{(1 - z)} \quad \text{or} \quad \phi = \frac{sY_F^0}{Y_O^0} \frac{sY_F - Y_0 + Y_0^0}{s(Y_F^0 - Y_F) + Y_O}
\]

Simple exercise: using Cantera, Cosilab or Chemkin

- Compute a 1D premixed flame with Lewis not equal for a chosen equivalence ratio \( \phi_1 \)
- Compute \( z = \frac{(sY_F - Y_0 + Y_0^0)}{(sY_F^0 + Y_0)} \)
- Plot \( z \) versus \( x \): it will be constant
- Compute the equivalence ratio from \( z \):

\[
\phi = \frac{sY_F^0}{Y_O^0} \frac{z}{(1 - z)}
\]

- And check it is equal to \( \phi_1 \)
- Repeat with real (non equal) values of Lewis numbers...
Will also work in 3D to know the local equivalence ratio in a code (useful for diffusion, partially premixed or spray flames):

**BEFORE COMBUSTION. EASY.** What is the equivalence ratio of the gases in the fresh gas?

\[ \phi = \frac{sY_F}{Y_O} \]

**AFTER COMBUSTION:** cant use the same formula. Compute \( z \) then get the equivalence ratio:

\[ \phi = \frac{sY_F^0}{Y_O^0} \frac{z}{(1 - z)} \]

---

**The limits of the \( z \) diagram**

- The concept of splitting the resolution of diffusion flame structures in two parts (\( z \) diagram and mixing problem) is common in many codes, even for turbulent diffusion flames.

- But can we really do this? can we base all our models on \( z \)? let us come back to the assumptions required to define a mixture fraction \( z \).
Equal Lewis numbers ??

- Never happens. Lewis numbers are not equal and not equal to unity. Lewis numbers measured in a 1D premixed flame.

**Alternative definitions for \( z \) ?**

- The literature contains multiple ‘improved’ definitions of \( z \) (based on elements, or on combination of elements).
- The mixture fraction defined using a single step global reaction is of course limited. For \( \text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O} \), define a mixture fraction \( z_1 \):

  \[
  z_1 = \frac{sY_{H_2} - Y_{O_2} + Y_{O_2}^0}{sY_{H_2}^0 + Y_{O_2}^0} = \frac{sY_{H_2} - Y_{O_2} + 1}{9}
  \]

- We know that this is not a good definition in practice since in the real world, we have more than one reaction.
- Solution: work on elements (C, H or O) because elements are always conserved. Generalized mixture fractions.
Other mixture fractions:

- For example, build a passive scalar on H atom:
  \[
  Z_H = W_H \left( \frac{2Y_{H_2}}{W_{H_2}} + \frac{Y_H}{W_H} + \frac{2Y_{H_2O}}{W_{H_2O}} + \frac{Y_{O_H}}{W_{O_H}} + \frac{Y_{HO_2}}{W_{HO_2}} + \frac{2Y_{H_2O_2}}{W_{H_2O_2}} \right)
  \]

- and a mixture fraction from it:
  \[
  z_H = \frac{Z_H - 0}{2Y_{H_2}^0 W_H/W_{H_2} - 0}
  \]

- See Bilger, Barlow, Pope's papers for other extensions. For example in the TNF workshop, Bilger’s definition is:
  \[
  z_B = \frac{2(Y_C-Y_{C,2})/w_C + (Y_H-Y_{H,2})/2w_H - (Y_O-Y_{O,2})/w_O}{2(Y_{C,1}-Y_{C,2})/w_C + (Y_{H,1}-Y_{H,2})/2w_H - (Y_{O,1}-Y_{O,2})/w_O}
  \]

But all mixture fractions are ... different:

- Measurements of various mixture fractions (based on C and H) in a piloted diffusion flame vs Bilger’s z:

[Graph showing measurements of mixture fractions]

R.S. Barlow et al. / Combustion and Flame 143 (2005) 433–449
Alternative definitions for $z$?

- In the end, ‘there is no such thing as a real mixture fraction’ because nothing (species or elements) diffuses at the same speed in a multispecies gas.

- This leads to multiple problems in practice since the multiple definitions of $z$ lead to $z$’s which are not equal...

Last comment on Lewis numbers

When we will discuss turbulent flames, we will see that many authors use unity Lewis number assumptions. Why?

- It seems to work better...

- It may be vaguely justified by the fact that small scale turbulence leads to turbulent transport which dominates transport and is the same for all species, thereby justifying the equal Lewis number assumption.
Stretch and scalar dissipation

- All previous derivations for premixed like diffusion cases use assumptions which are too simple. In practice, at least one additional notion is required for turbulent flames: stretch.
- Stretch applies to any flame (premixed or diffusion) and measures the rate at which the flame area increases:

\[ \kappa = \frac{1}{A} \frac{dA}{dt} \]

- Intuition tells us that ‘stretching’ a flame must have a limit. The flame is affected by stretch (see Williams book or Pr Matalon’s course).
- This effect is different for premixed and diffusion flames.

Stretch and premixed flames

\[ \kappa = \nabla_t \cdot \vec{u} - s_d \left( \frac{1}{R_1} + \frac{1}{R_2} \right) = \nabla_t \cdot \vec{u} + s_d \nabla_t \cdot \vec{n} \]

- Strain in the tangent plane to the flame
- Strain due to flame propagation
- Displacement speed
- Front curvature

Examples of stretched premixed flames

Evaluations of stretch:

\[ \kappa = \frac{U_1 + U_2}{d} \]

This is an average value: stretch is not constant along the flame normal
Defining flame stretch at the flame location is difficult
Flame location in a stagnation point flow:

- Flame thickness

Evaluations of stretch: spherical flames

\[ A = 4\pi r^2 \]

\[ \kappa = \frac{1}{A} \frac{dA}{dt} = \frac{2}{r} \frac{dr}{dt} \]

Stretch is constant on the flame front
Knowing \( r(t) \) gives directly stretch
Stretch changes like \( 1/r \): very large at initial times
**Variations of flame speeds with stretch**

- Premixed flames are affected by stretch.
- Theory can be used to derive the variations of speeds:

  \[
  \frac{s_d(0)}{s^0_L} = 1 - \frac{L_a^d}{s^0_L} \kappa
  \]

  \[
  \frac{s_a(0)}{s^0_L} = 1 - M_a^d \frac{\kappa \delta}{s^0_L}
  \]

- Measuring Markstein numbers is extremely difficult...
- But the dependence of premixed flame speeds on stretch is not very strong, compared to diffusion flames

**Flame speeds versus stretch: depend on the Lewis number of the deficient reactant AND on heat losses:**

![Diagram showing flame speeds versus stretch](Image)

- *ADIABATIC Lewis=1*
**ADIABATIC Lewis < 1**

\[ s_c = s_L^0 \cdot L_a C K \]

**NON ADIABATIC Lewis > 1**

\[ s_c = s_L^0 \cdot L_a C K \]

---

**Stretch and diffusion flames:**

In diffusion flames, flame strain is often replaced by a more useful quantity called ‘scalar dissipation’:

\[ \chi = 2D \left( \frac{\partial z}{\partial x_i} \frac{\partial z}{\partial x_i} \right) \]

Why?
- Scalar dissipation does not depend on the flame orientation (as flame stretch does).
- For simple cases (stretched diffusion flame), stretch and scalar dissipation are directly linked.
The diffusion flame with infinitely fast chemistry:

\[ \phi = s \frac{Y_F^0}{Y_O^0} \]

Flame stretch

\[ \chi_f = \frac{a}{\pi} \exp \left[ -2 \left( \text{erf}^{-1} \left( \frac{\phi - 1}{\phi + 1} \right) \right)^2 \right] \]

Scalar dissipation on the flame front

We can work with stretch OR with scalar dissipation

Figure 6.5.2. Calculated velocity and temperature profiles for a symmetric, nozzle-generated counterflow flame established by impinging a 23 percent methane-in-nitrogen stream against a 23 percent oxygen-in-nitrogen stream, for different descriptions of the flow (Sung, Liu & Law 1995).
Diffusion flames are VERY sensitive to stretch (or scalar dissipation)

\[
\dot{\Omega}_F = -\rho \frac{Y_F^0}{1 - \zeta_{st}} \sqrt{\frac{aD}{2\pi}} e^{-\zeta_f^2}
\]

When you stretch a diffusion flame, it burns more: we all know we must blow on fires...: we just bring them more air

If you stretch it too much, you can quench it: we also know that you should not blow too much on a candle, otherwise you kill it...

---

Stretching a diffusion flame:

Total fuel consumption

- Scalar dissipation at stoichiometric point ($\chi_{st}$)
- Flame strain ($\alpha$)
- Inverse Damköhler ($D^{-1}$)
Implications for turbulent flames:

- In turbulent flames, the unsteady velocity field will induce strain and therefore stretch:

\[
\kappa = \nabla_t \cdot \mathbf{u} - s_d \left( \frac{1}{R_1} + \frac{1}{R_2} \right) = \nabla_t \cdot \mathbf{u} + s_d \nabla_t \cdot \mathbf{n}
\]

\(\kappa\) Strain in the tangent plane to the flame
\(s_d\) Strain due to flame propagation

In turbulent flames:

- We will need to establish a link between the velocity field (created by an ensemble of vortices) and the flame stretch:

\[
\kappa = \nabla_t \cdot \mathbf{u} - s_d \left( \frac{1}{R_1} + \frac{1}{R_2} \right) = \nabla_t \cdot \mathbf{u} + s_d \nabla_t \cdot \mathbf{n}
\]
Are all flames premixed or non-premixed?

No and two other cases must be mentioned:
- triple flames
- partially premixed flames

TRIPLE FLAMES: THE STRUCTURE WHICH SEPARATES IGNITED FROM NON IGNITED DIFFUSION LAYERS

In any flame where you inject pure fuel and pure oxidizer, you can be either on the mixing line or on the combustion line. How do you go from one to the other? (in other words: how do you ignite a diffusion flame?)
TRIPLE FLAMES: THE STRUCTURE WHICH SEPARATES IGNITED FROM NON IGNITED DIFFUSION LAYERS

Fuel → Oxidizer

MIXING STATE

Kioni flame

Oxidizer → Fuel

BURNING STATE

TRIPLE FLAME POINTS IN A z DIAGRAM:

MIXING STATE

Infinitely fast chemistry

Diffusion flame

Premixed zone

Lean premixed flame

Rich premixed flame

Fuel → Oxidizer

Mixing lines

Fuel mass fraction

Mixture fraction
1/ TRIPLE FLAMES PROPAGATE.
2/ THEY PROPAGATE FASTER THAN PREmixed FLAMES

- A TRIPLE FLAME SPEED SCALES LIKE:

\[ s_{Triple} = s^0_L \sqrt{\frac{\rho_1}{\rho_2}} \]

Stoechiometric laminar flame speed
Density ratio

Partially premixed flames
- Almost noone uses perfectly premixed flames: too dangerous
- And almost noone uses pure diffusion flames: not efficient
- Most flames will be produced in devices where we TRY to mix at the last moment to reach premixed conditions but never really make it.... Partially premixed flames

Mean equivalence ratio
Real distribution on flame front
Example: the PRECCINSTA burner (DLR)