# Combustion in Low Mach Isotropic Turbulence

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# Introduction



Analysis of interaction between chemical kinetics and turbulent flow in the simplest conditions as possible

ideal geometry: periodic box ۲

> spectral method for calculation and Fourier data analysis -

- real physics: Direct Numerical Simulation (DNS) ۲
  - All the scales are correctly simulated
  - The interaction is exactly described -

# Statistical steadiness

Homogeneity and isotropy implies:

- Independence of statistics from rotation or position
- Simple scale-by-scale analysis
- Statistical steady state
  - Ensemble averages are replaced by spatial-temporal averages
  - Time independent energy budget
- How to do this? —> Forcing on the largest scales

 Advances in turbulence have been achieved by homogeneous and isotropic conditions (e.g. K-41 theory)

# Typical conditions and simplifying assumptions

Main properties of a turbulent deflagrative flame:

- Flow velocity is lower than the sound speed because of high temperature
- The essential feature of turbulent combustion is the variation of density and of molecular diffusions with temperature
- Single scale low Mach asymptotic set of equations:
  - It permits to calculate variable density flows
  - There is not a cancellation error to evaluate the pressure gradient
  - It avoids the numerical stiffness related to the time step of a fully compressible scheme

### Governing equations

After a single scale asymptotic expansion on low Mach number, the set of non dimensional equations become:

$$\begin{split} \frac{\partial \rho_0}{\partial t} + \nabla \cdot (\rho \, u)_0 &= 0 \\ \frac{\partial (\rho \, u)_0}{\partial t} + \nabla \cdot (\rho \, u \, u)_0 &= \frac{1}{Re} \, \nabla \cdot \tau_0 - \nabla \, p_2 \\ \frac{\partial (\rho \, Y_a)_0}{\partial t} + \nabla \cdot (\rho \, u \, Y_a)_0 &= \frac{1}{Re \, Sc_a} \, \nabla \cdot (\mu \, \nabla \, Y_a)_0 + Da_a \, \omega_{a0} \\ \frac{dp_0}{dt} + \gamma \, p_0 \, \nabla \cdot u_0 &= \frac{\gamma}{Re \, Pr} \, \nabla \cdot (k_0 \, \nabla \, T_0) + (\gamma - 1) \sum_a Da_a \, Ce_a \, \omega_{a0} \\ T_0 &= \frac{p_0}{\rho_0} \end{split}$$

where:  $f(x,t) = f_0(x,t) + f_2(x,t)M^2 + O(M^3)$ 

# Integration technique

- Pseudo-spectral method with dealiasing techniques is used for spatial discretization
  - Excellent accuracy with regular functions
  - No wavenumber modification or phase error
  - Time integration is performed by an explicit Runge-Kutta method
    - Fourth order time accuracy
    - Low-storage scheme

# Pressure evaluation

#### State of art:

- Projection methods
- Pressure correction methods
- Semi-implicit methods
- Method requirements:
  - Stability for large density differences which occurs in combustion
  - Accuracy to preserve global forth order scheme in time
- Present projection iterative technique:
  - Possibility to control the iteration error
  - Fast and accurate for periodic geometry and for combustion conditions
  - Fully integrated in the low-storage Runge-Kutta scheme

# Iterative technique (1)

Decompose the momentum as:  $(\rho u) = (\rho v) + \nabla \phi$  hence the equation for  $(\rho v)$  follows:

$$\frac{\delta(\rho v)}{\delta t} = \nabla \cdot \left[ -(\rho u u) + \frac{1}{Re} \tau \right]$$

• Through comparison between momentum and  $(\rho v)$  equations:

$$\phi = \int_{\delta t} p_2 dt + c$$

The equation for  $\phi$  is obtained by enforcing the value of  $\nabla \cdot u^{k+1}$  given by the energy equation

$$\nabla^2 \phi^{k+1} = \rho^{k+1} \nabla \cdot u^{k+1} - \nabla \cdot (\rho v)^{k+1} + \underline{u^{k+1}} \cdot \nabla \rho^{k+1}$$

All r.h.s. terms are known except  $u^{k+1}$ 

## Iterative technique

The semi-discrete set of equations evolved by Runge-Kutta:

$$\begin{aligned} \frac{\delta \rho}{\delta t} &= -\nabla \cdot (\rho u) \\ \frac{\delta (\rho v)}{\delta t} &= \nabla \cdot \left[ -(\rho u u) + \frac{1}{Re} \tau \right] \\ \frac{\delta (\rho Y_a)}{\delta t} &= \nabla \cdot \left[ -(\rho u Y_a) + \frac{1}{ReSc_a} \nabla \cdot (\mu \nabla Y_a) \right] + Da_a \omega_a \\ \frac{\delta p}{\delta t} &= (\gamma - 1) \sum_a Da_a Ce_a \frac{1}{V} \int_V \omega_a dV \\ \nabla \cdot u &= \frac{1}{p} \left[ \frac{1}{RePr} \nabla \cdot (k \nabla T) + \frac{\gamma - 1}{\gamma} \sum_a Da_a Ce_a \left[ \omega_a - \frac{1}{V} \int_V \omega_a \right] \right] \\ T &= \frac{p}{\rho} \end{aligned}$$

# Iterative technique (2)

The iterative algorithm for  $\phi^{k+1}$ :

first iteration:

$$u^{I} = v^{k+1}$$
$$\nabla^{2} \phi^{I} = \rho^{k+1} \nabla \cdot u^{k+1} - \nabla \cdot (\rho v)^{k+1} + u^{I} \cdot \nabla \rho^{k+1}$$

successive approximations:

$$u^{s} = v^{k+1} + \frac{\nabla \phi^{s-1}}{\rho^{k+1}}$$
$$\nabla^{2} \phi^{s} = \rho^{k+1} \nabla \cdot u^{k+1} - \nabla \cdot (\rho v)^{k+1} + u^{s} \cdot \nabla \rho^{k+1}$$

When  $||u^s - u^{s-1}|| \le \epsilon$ , the iterative procedure is stopped giving the momentum field:

 $(\rho u)^{k+1} = (\rho v)^{k+1} + \nabla \phi^s$ 

# Test for iterative technique

- Two plane flame front propagating in the periodic box
  - The initial momentum field is null
  - One-step reaction with three chemical species namely  $F+O \rightarrow P$
  - Reactants are fully premixed
  - 1-D Gaussian heat source is used to start chemical reactions
  - After the 'spark' the temperature ratio is about 20



### Iterative procedure convergence

To evaluate the error decay as function of iteration the infinity norm is adopted:  $err^{s} = ||u^{s} - u^{s-1}||_{\infty}$ ,  $s = 2...N_{max}$ 



### Physics of the simulated box



Turbulent kinetic energy is introduced at the largest scales

The large scale vortices transports chemical species and related enthalpy inside or outside the box

Statistically steadiness in the periodic box

The energy injection is simulated by a random forcing in the momentum equation:

$$\rho f_i = \sqrt{\rho} \left[ A(t)_{ij} \sin(x_j) + B(t)_{ij} \cos(x_j) \right]$$

- Acts on the largest scales
- Only rotational component of kinetic energy is stirred
- $A(t)_{ij}, B(t)_{ij}$  are random function with gaussian distribution in time

Large scale species mixing and injection is simulated via random forcing in the equation of chemical species:

$$\frac{\partial (\rho Y_a)}{\partial t} + \nabla \cdot (\rho u Y_a) = \frac{1}{Re Sc_a} \nabla \cdot (\mu \nabla Y_a) + Da_a \omega_a + \underline{f}_a$$
$$f_a = A_a [1 + \sin(x + \theta(t))]$$

Provides reactants and remove products

- The large scale mixing is guaranteed by the random phase  $\theta(t)$ 

Finally the mean value of internal energy is kept constant

## Steady state combustion (1)

Two simulations are performed with almost the same fluid dynamics parameters but with different chemical kinetics



## Steady state combustion (2)

The chemical kinetics parameters show different mean values



### Characteristic non dimensional parameters

Turbulence times: 
$$t_0 = \frac{l_0}{U_{rms}}$$
  $t_\eta = \frac{\eta}{u_\eta}$ 

Chemical kinetics time:  $t_c = \frac{\rho_p}{\omega_p}$ 

Interaction:

$$Ka = \frac{t_c}{t_\eta} = \frac{\delta_L^2}{\eta^2} \qquad Da_t = \frac{t_0}{t_c} = \frac{\omega_p l_0}{\rho_p u_{rms}}$$

$$Re = Ka^2 Da_t^2$$





Simulation F shows some propagating 'flame fronts'

# Scale-by-scale energy budget (1)

The momentum equation may be written in terms of the variable:  $w = \sqrt{\rho} u$ 

$$\frac{\partial w}{\partial t} = -\left(u \cdot \nabla w + \frac{1}{2}(\nabla \cdot u)w\right) - \frac{1}{\sqrt{\rho}}\nabla p + \frac{1}{\sqrt{\rho}}\nabla \cdot \tau + \sqrt{\rho}f$$

Using the decomposition:  $w = w_r + w_c$ 

such that:  $\nabla \times w_c = 0$ ,  $\nabla \cdot w_r = 0$ 

is possible to write the equations for the rotational and compressive components of kinetics energy in Fourier space:

$$\begin{split} \left[ \frac{\partial \hat{w}}{\partial t} \right] \cdot \hat{w}_{i} = \left[ -\left( u \cdot \nabla w + \frac{1}{2} (\nabla \cdot u) w \right) - \frac{1}{\sqrt{\rho}} \nabla p + \frac{1}{\sqrt{\rho}} \nabla \cdot \tau + \sqrt{\rho} f \right]^{2} \cdot \hat{w}_{i} \\ \frac{\partial \hat{E}_{i}(k)}{\partial t} = -\left( u \cdot \nabla w + \frac{1}{2} (\nabla \cdot u) w \right)^{2} \cdot \hat{w}_{i} - \left( \frac{1}{\sqrt{\rho}} \nabla p \right)^{2} \cdot \hat{w}_{i} + \left( \frac{1}{\sqrt{\rho}} \nabla \cdot \tau \right)^{2} \cdot \hat{w}_{i} + \left( \sqrt{\rho} f \right)^{2} \cdot \hat{w}_{i} \quad i = r, c \\ \frac{\partial \hat{E}_{i}(k)}{\partial t} = \hat{NL}_{i}(k) + \hat{P}_{i}(k) + \hat{V}_{i}(k) + \hat{F}_{i}(k) \quad i = r, c \end{split}$$

since:  $\hat{w}_r(k) \cdot \hat{w}_c(k) = 0$ 



#### S simulation

F simulation

## Scale-by-scale scalar budget (1)

As far as for kinetic energy equation, a budget is done for scalar equation:

$$\frac{\partial \hat{\rho}_a}{\partial t} \hat{\rho}_a = \left[ -\nabla \cdot (\rho_a u)^{\hat{}} + \frac{1}{Re Sc_a} \nabla \cdot (\mu \nabla Y_a)^{\hat{}} + Da_a \hat{\omega}_a \right] \hat{\rho}_a$$

$$\frac{\partial \hat{E}_{\rho_a}(k)}{\partial t} = N\hat{L}_{\rho_a}(k) + \hat{V}_{\rho_a}(k) + R\hat{R}_{\rho_a}(k) + \hat{F}_{\rho_a}(k)$$

### Scale-by-scale scalar budget (2)



# Final Remarks

Accurate iterative pressure solver for low Mach number flows

In statistically steady state combustion we have discussed:

- Scale-by-scale budget for compressive and rotational kinetic energy
- Scale-by-scale budget for scalar fields

#### Future work

- Multiple scale expansion to take into account acoustical effects
- Detailed chemical kinetics
- Benchmarking for LES calculation