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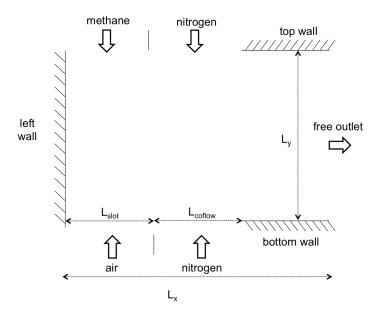
TC5- Numerical methods

Master PPF

Final project: combustion of methane in a counterflow configuration

1 Configuration

The configuration consists of two diametrically opposed injections: one injecting pure methane, and the other injecting pure air, both at 300~K. Experimentally, a co-current of N_2 is often used to dilute the burnt gases, and to protect the zone of interest from the variations of the external flow. The geometrical details of the configuration are given in Fig. 1.



The dimensions are:

| L_x | L_y | L_{slot} | L_{coflow} |
|-------|-------|------------|--------------|
| 2 mm | 2 mm | $0.5 \ mm$ | 0.5~mm |

Velocity and temperature at injection are:

| U_{slot} | T_{slot} | U_{coflow} | T_{coflow} |
|----------------|------------|------------------|--------------|
| $1 \ m.s^{-1}$ | 300~K | $0.2 \ m.s^{-1}$ | 300~K |

Finally, we will consider pure methane for the upper injection, and pure air for the lower injection, the co-current being composed of pure nitrogen.

2 Equations

2.1 Fluid flow

We consider the two-dimensional flow of a Newtonian fluid with constant density and viscosity. The velocity components u and v verify the Navier-Stokes equations, in addition to the conservation of mass equation:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$
$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right)$$
$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

where $\rho = 1.1614~kg.m^{-3}$ is the fluid density et $\nu = 15 \times 10^{-6}~m^2.s^{-1}$ is the kinematic viscosity.

2.2 Species and temperature

$$\begin{split} \frac{\partial Y_k}{\partial t} + u \frac{\partial Y_k}{\partial x} + v \frac{\partial Y_k}{\partial y} &= D \left(\frac{\partial^2 Y_k}{\partial x^2} + \frac{\partial^2 Y_k}{\partial y^2} \right) + \frac{\dot{\omega}_k}{\rho} \\ \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} &= a \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \frac{\dot{\omega}_T}{\rho c_n} \end{split}$$

with k the index identifying each species. We will consider here unity Schmidt and Prandtl numbers $(D=a=\nu)$. The mass heat capacity of the fluid will be assumed to be constant and of value $c_p=1200~J.kg^{-1}.K^{-1}$.

2.3 Chemistry of methane

We are interested in a one-step chemistry of methane combustion in air:

$$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2$$

The progress rate of the reaction is written following Arrhenius law:

$$Q = A[CH_4][O_2]^2 \exp\left(-\frac{T_a}{T}\right)$$

where $T_A=10000K$ and $A=1.1\times 10^8~[SI~units]$. $[CH_4]$ et $[O_2]$ are respectively the concentrations in CH_4 et en O_2 ($[k]=\rho \frac{Y_k}{W_k}$). The reaction rate $\dot{\omega}_k$ of species k is:

$$\dot{\omega}_k = W_k \nu_k Q$$

where W_k is the molar mass of species k, et ν_k is the molar stoichiometric coefficient, which are given in the table below:

| ν_{CH_4} | ν_{O_2} | ν_{N_2} | ν_{H_2O} | $ u_{CO_2}$ |
|--------------|-------------|-------------|--------------|-------------|
| -1 | -2 | 0 | 2 | 1 |

The heat release is finally expressed here as:

$$\dot{\omega}_T = -\sum_{k=1}^{N_S} \frac{\Delta h_{f,k}^0}{W_k} \dot{\omega}_k$$

where $\Delta h_{f,k}^0$ is the enthalpy of formation of species k. Values are given in the table below:

| $\Delta h_{f,N_2}^0$ | $\Delta h_{f,O_2}^0$ | $\Delta h_{f,CH_4}^0$ | $\Delta h_{f,H_2O}^0$ | $\Delta h_{f,CO_2}^0$ |
|----------------------|----------------------|-----------------------|-----------------------|-----------------------|
| $0 \ kJ/mol$ | $0 \ kJ/mol$ | $-74.9 \ kJ/mol$ | $-241.818 \ kJ/mol$ | $-393.52 \ kJ/mol$ |

3 Questions

We are here solely interested in the steady solutions

3.1 Flow field

We first study the flow without combustion. We will consider that the left wall is a slipping wall ("free" tangential velocity), while the other walls are non-slipping. To solve this flow, we will use a fractional-step method.

• What is the maximum strain rate a on the left slipping wall? (a $=\left|\frac{\partial v}{\partial y}\right|$)

3.2 Species transport

We now add species transport. However, neither combustion nor temperature transport will be activated.

• Measure the thickness of the diffusive zone on the left wall using the N_2 species. This thickness will be taken as that of the zone between $\mathbf{Y_{N_2}} \in [\mathbf{10\%Y_{N_2}^{slot}}, \mathbf{90\%Y_{N_2}^{slot}}]$.

3.3 Combustion

Now we want to activate the combustion. For this, several steps are recommended:

3.3.1 Simulation of an homogeneous reactor

In order to deal with the time scales and complexity of solving the chemistry, implement a function that integrates the chemical source terms between time t_0 and $t_0 + \tau$. The system of equations to solve is

$$\frac{\mathrm{d}Y_k}{\mathrm{d}t} = \frac{\dot{\omega}_k}{\rho},$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\dot{\omega}_T}{\rho c_p}.$$

It can be considered with the temperature evolution T(t) or in a first case with T=cte, corresponding to a homogeneous isothermal reactor. For given initial conditions (air+fuel), and beyond a certain temperature ($\simeq 1000 \mathrm{K}$), the mixture will auto-ignite. With an explicit method, this steep process requires a very small time step Δt_{chem} to ensure the stability of the system.

3.3.2 Ignition of the flame for a frozen temperature field

Being interested in the stationary state of the system, it is not necessary to capture faithfully the ignition and its evolution. To ignite the flame, the temperature field T(x,y) is in a first step frozen in time. To ensure the ignition, you can impose in a band centered around the stagnation plane and of thickness $\delta = 0.5mm$ a temperature of $1000 \mathrm{K}$ ($300 \mathrm{K}$ outside this band). This allows to initiate the combustion. In your scalar advection-diffusion code, you will apply in each of the space the time integration of the chemical terms between the current time t and the next time $t + \Delta t$ from the function developed above. Note that Δt_{chem} is independent of $\tau = \Delta t$. To speed up the calculation, it may be relevant to use the vectorization capabilities of Matlab or Python (by applying your function directly on the 2D fields and not index by index).

3.3.3 Flame with resolved temperature equation

Once the flame is stabilized under the previous conditions, activate the complete solution of the temperature equation (advection, diffusion, reaction) coupled with the rest of the equations.

• What is the maximum temperature?