

DISCUSSION ABOUT A MIXING AND REACTING FLOW MODEL FOR COMBUSTION

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Abstract The aim of this work is the numerical solution of mixing and reacting flows with fuel consumption. The model approximates the overall, single step, binary, irreversible reaction between two species, resulting a third, which is taken to be a process of first order with respect to each of the reactants, being the specific reaction rate controlled by temperature-dependent Arrhenius kinetics. The simulations are performed using the finite differences explicit Runge-Kutta five-stages scheme for third order time and fourth order space approximations. Consistent results are obtained, showing that the model is able to follow nonlinear behavior of the mixing and reaction progress, for Schmidt and Prandtl numbers of order 1, Zel'dovich 10, Damköhler 300 and heat release parameter 10, which are reasonable values for gaseous hydrocarbon chemistry.

Keywords: Mixing Flows, Reacting Flows, Combustion Model, Numerical Simulation, Parameters influence

1. Introduction

Practical applications, such as combustion, involve the analysis of mixing and reacting flows. The process of combustion is highly complex, including heat transfer, chemistry, combustion and also radiation; it is an important multidisciplinary topic of research.

Combustion involves a large range of time and length scales; small turbulence scales have small times because of viscous dissipation, having limited effects on combustion. Scales such as the vorticity diffusion length, $\lambda_v \sim \delta R_e^{-3/4}$, where δ is the thickness, the molecular diffusion length, $\lambda_D \sim \lambda_v S_c^{-1/2}$, and the characteristic length, $\lambda_r \sim \lambda_D D_a^{-1/3}$, turn finer with the increase of Reynolds, R_e , Schmidt, S_c , and Damköhler, D_a , numbers, causing severe numerical resolution restrictions.

The propagation of a flame strongly depends on the quality of reactants mixing. For an organized jet motion, as shown in Fig. 1, the evolution of large scale structure is governed by Kelvin-Helmholtz instabilities; frequency and energy distribution among the length scales is controlled by the initial conditions of the flow (Renard et al., 2000).

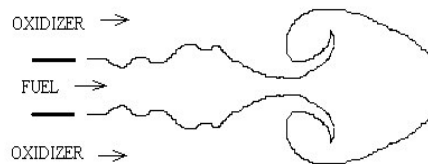


Fig. 1 Flame-vortex interaction

The present work develops a numerical technique for mixing and reacting flow inside a turbine model. A theoretical model to couple fluid dynamics, heat transfer and chemical kinetics is presented. Some computations are performed for reasonable values for hydrocarbon chemistry, to focus the effect of product formation. The numerical technique is based on the finite difference explicit Runge-Kutta five-stages scheme and the virtual boundary method.

2. Governing equations

The set of non-linear governing equations for mass, momentum, energy and chemical species is following indicated. The model is based on the one-step finite rate Arrhenius kinetics (Wang et al., 1999)



and chemistry is considered to be infinitely fast.

As the reaction heat release is supposed to be known and the temperature changes are significant, it is sufficient to predict the overall structure of the flame, resulting, after simplification, the set of mass averaged, Favre filtered, $\tilde{f} = \overline{\rho f} / \bar{\rho}$, governing equations for (De Bortoli, 2003-2004) :

Mass conservation

$$\frac{\partial \bar{p}}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_j)}{\partial x_j} = 0 \quad (2)$$

Momentum

$$\frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}}{R_e} \tilde{\tau}_{ij} \right) + \frac{\partial}{\partial x_j} \left(\frac{\mu_T}{R_{eT}} \tilde{\tau}_{ij} \right) + \tilde{F}_i \quad (3)$$

Energy

$$\frac{\partial (\bar{\rho} \tilde{T})}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{T})}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\bar{\mu}}{R_e P_r} \frac{\partial \tilde{T}}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left(\frac{\mu_T}{R_{eT} P_{rT}} \frac{\partial \tilde{T}}{\partial x_i} \right) + v_p H_e \bar{w} \quad (4)$$

Chemical Species

$$\frac{\partial (\bar{\rho} \tilde{C}_k)}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{C}_k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\bar{\mu}}{R_e S_c} \frac{\partial \tilde{C}_k}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left(\frac{\mu_T}{R_{eT} S_{cT}} \frac{\partial \tilde{C}_k}{\partial x_i} \right) \mp v_k \bar{w} \quad (5)$$

where $\tilde{\tau}_{ij} = \tilde{S}_{ij} - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k}$ is the strain tensor, $\tilde{S}_{ij} = \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}$ the mean strain rate, $\bar{w} = D_a (\bar{\rho} \tilde{C}_f) (\bar{\rho} \tilde{C}_o) e^{-Z/T}$ the reaction rate, $\bar{\mu} \sim \tilde{T}^{3/4}$ the viscosity, $\mu_T = \bar{\rho} C \Delta^2 |\tilde{S}|$ the eddy viscosity with $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$ and $F_i = G_r \rho \Delta \tilde{T} / R_e^2$ the bouyancy term with $\Delta \tilde{T}$ the temperature increase, G_r the Grashof and R_e the Reynolds. P_r is the Prandtl, Z the Zel'dovich and H_e the heat release parameters. Product $R_e P_r = P_e$ is the Peclet number and $R_e S_c = L_e$ the Lewis number, the ratio of thermal and species diffusivity. D_a is the Damköhler number, a ratio between the mechanical and chemical time. The \mp sign refers to the reactant consumption and product formation, respectively; $C=0.1$ is a constant and Δ the subgrid characteristic length scale. Observe that chemical source terms change considerably, they are exponential functions of the temperature. Turbulent Reynolds number, $R_{eT} = D_a^2 K_a^2$, depends on the Karlovich number, K_a ; in this work $K_a < 1$.

The incognits are the mixture density ρ , the fluid velocities u_i , the temperature T , the chemical species C_f , C_o and C_p and the pressure p . Pressure can be obtained using the state relation

$$\bar{p} = \bar{\rho} R \tilde{T} \quad (6)$$

3. Solution Procedure

Nowadays, the tendency seems to be the solution of turbulent flows using DNS – Direct Numerical Simulation or LES – Large Eddy Simulation instead of RANS – Reynolds Averaged Navier-Stokes technique (see Fig. 2). DNS is limited to low Reynolds numbers and simplified geometries because of high resolution requirements and associated computational costs (Poinsot et al., 1996; Boersma, 1998). With LES large scales are resolved while the small scales are by a subgrid model modeled. It occupies an intermediate position between the DNS and RANS (Veynante and Poinsot, 1996; Boersma and Lele, 1999; Stone and Menon, 2003).

Besides, a theoretical/analytical analysis is always desired to give confidence to the numerical simulations. Recently, Zavaleta Calderón et al (2003) established the existence of a unique classical solution considering a weak coupling of the reactants via advection by an independently developing velocity and proved the existence and uniqueness of the solution via a semigroup formulation and the maximum principle.

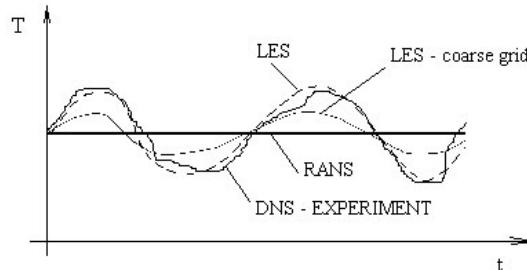


Fig. 2 Schematic comparison of numerical simulation techniques

When the central finite differences scheme is employed, for a point (i,j) (see figure 3 for details) in the computational domain, results the following fourth order space derivative approximations for a general variable ψ (Anderson et al., 1984)

$$\frac{\partial \psi}{\partial x} = \frac{\psi_{i-2,j} - 8\psi_{i-1,j} + 8\psi_{i+1,j} - \psi_{i+2,j}}{12\Delta x} \quad (7)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-\psi_{i-2,j} + 16\psi_{i-1,j} - 30\psi_{i,j} + 16\psi_{i+1,j} - \psi_{i+2,j}}{12\Delta x^2} \quad (8)$$

and similarly for other derivatives. After a simplification and numerical approximation, results the following form for energy equation for Runge-Kutta time-stepping scheme, as example

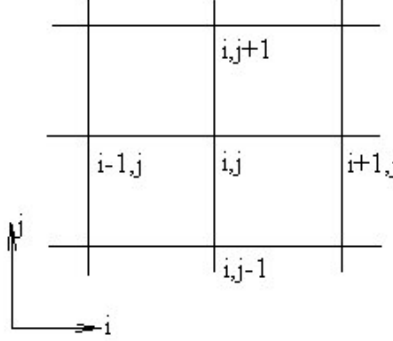


Fig. 3 Conventional cartesian grid

$$\begin{aligned} \frac{\partial(\tilde{\rho}\tilde{T})}{\partial t} \Big|_{i,j} = & \frac{(\tilde{\rho}\tilde{u}\tilde{T})_{i-2,j} - 8(\tilde{\rho}\tilde{u}\tilde{T})_{i-1,j} + 8(\tilde{\rho}\tilde{u}\tilde{T})_{i+1,j} - (\tilde{\rho}\tilde{u}\tilde{T})_{i+2,j}}{12\Delta x} - \frac{(\tilde{\rho}\tilde{v}\tilde{T})_{i,j-2} - 8(\tilde{\rho}\tilde{v}\tilde{T})_{i,j-1} + 8(\tilde{\rho}\tilde{v}\tilde{T})_{i,j+1} - (\tilde{\rho}\tilde{v}\tilde{T})_{i,j+2}}{12\Delta y} + \\ & \frac{E_{i-2,j} - 8E_{i-1,j} + 8E_{i+1,j} - E_{i+2,j}}{12\Delta x} + \frac{F_{i,j-2} - 8F_{i,j-1} + 8F_{i,j+1} - F_{i,j+2}}{12\Delta y} + \\ & \frac{E_{T_{i-2,j}} - 8E_{T_{i-1,j}} + 8E_{T_{i+1,j}} - E_{T_{i+2,j}}}{12\Delta x} + \frac{F_{T_{i,j-2}} - 8F_{T_{i,j-1}} + 8F_{T_{i,j+1}} - F_{T_{i,j+2}}}{12\Delta y} + v_p H_e D_a \left[\rho C_f \rho C_o e^{-Z/T} \right]_{i,j} \end{aligned} \quad (9)$$

with

$$E_{i,j} = \left(\frac{\mu}{R_e P_r} \right)_{i,j} \frac{\tilde{T}_{i-2,j} - 8\tilde{T}_{i-1,j} + 8\tilde{T}_{i+1,j} - \tilde{T}_{i+2,j}}{12\Delta x}; \quad E_{T_{i,j}} = \left(\frac{\mu_T}{R_{eT} P_{rT}} \right)_{i,j} \frac{\tilde{T}_{i-2,j} - 8\tilde{T}_{i-1,j} + 8\tilde{T}_{i+1,j} - \tilde{T}_{i+2,j}}{12\Delta x} \quad (10)$$

$$F_{i,j} = \left(\frac{\mu}{R_e P_r} \right)_{i,j} \frac{\tilde{T}_{i,j-2} - 8\tilde{T}_{i,j-1} + 8\tilde{T}_{i,j+1} - \tilde{T}_{i,j+2}}{12\Delta y}; \quad F_{T_{i,j}} = \left(\frac{\mu_T}{R_{eT} P_{rT}} \right)_{i,j} \frac{\tilde{T}_{i,j-2} - 8\tilde{T}_{i,j-1} + 8\tilde{T}_{i,j+1} - \tilde{T}_{i,j+2}}{12\Delta y} \quad (11)$$

The other equations are approximated in a similar manner; they are solved after the application of the boundary conditions.

3.1 Boundary conditions

The proper implementation of boundary conditions is always important when solving flow problems. Although velocities are equal to zero at solid boundaries, density, pressure, temperature and chemical specie values must be known or estimated. Extrapolations (of the same order of domain discretization) are an alternative when we don't know the real value of a variable; usually not all variables are extrapolated because of code stability restrictions. Therefore, the boundary conditions can be summarized, without bars, as follows for (see Fig. 4):

- walls: no slip flow
- inlet: air supply C_o for fuel

outlet: variables extrapolation

injection: fuel C_f injected with a parabolic profile ($u_{\max} = 1$)

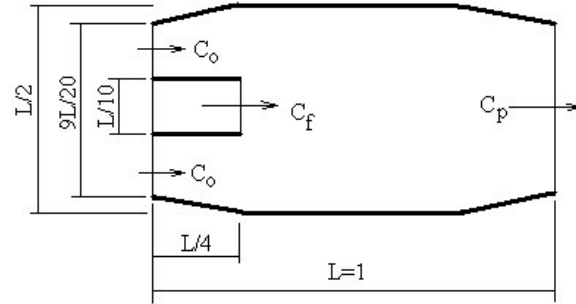


Fig. 4 Geometry for turbine model

As one see in (Fig. 4), the conditions are of Dirichlet or Neumann types. Their implementation in general do not maintain the higher order adopted at spatial discretization, as could be expected.

3.2 Time-stepping scheme

To obtain numerical solutions of high accuracy, the low storage Runge-Kutta method is chosen. This method is characterized by its low operation count and low storage requirements. More than two stages are employed to extend the stability region. Therefore, the following multistage scheme is employed

$$\begin{aligned}\bar{W}_{i,j}^{(0)} &= \bar{W}_{i,j}^{(n)} \\ \bar{W}_{i,j}^{(r)} &= \bar{W}_{i,j}^{(0)} - \alpha_r \Delta t \bar{R}_{i,j}^{(r-1)} \\ \bar{W}_{i,j}^{(n+1)} &= \bar{W}_{i,j}^{(r)}\end{aligned}\tag{12}$$

where $\bar{R}_{i,j}$ corresponds to the residuum, with $r = 0,1,2,3,4(n=5)$. \bar{W} is the vector of flux variables given by $\bar{W} = [\bar{\rho}, \bar{\rho}\tilde{u}, \bar{\rho}\tilde{v}, \bar{\rho}\tilde{T}, \bar{\rho}\tilde{C}_f, \bar{\rho}\tilde{C}_o, \bar{\rho}\tilde{C}_p]^T$ and the pressure p comes from the state relation.

When using explicit methods, time-step restrictions are natural; however, small time-steps are needed to well represent the mixture/reaction time scales. There are many discussions about the employment of explicit and implicit methods for transient and turbulent problems such as combustion. The choose for time and space approximations here follow simplicity reasons and the numerical results seem to be coherent.

4. Numerical results

Following, numerical results for the flow inside a turbine model is shown for small times, $t \leq 1s$. Time steps are of order $10^{-5}-10^{-6}$ and the computational mesh is still coarse, 161×87 points. Fig. 5 and 6 show the vortex formation; vortex motion controls the mixing, specially the large-scale vortices developing in the highly sheared regions of the flow. Vortex structures can also indicate a flow instability (Renard et al., 2000). Fig. 6 follows the organized flame-vortex motion presented in Fig. 1.

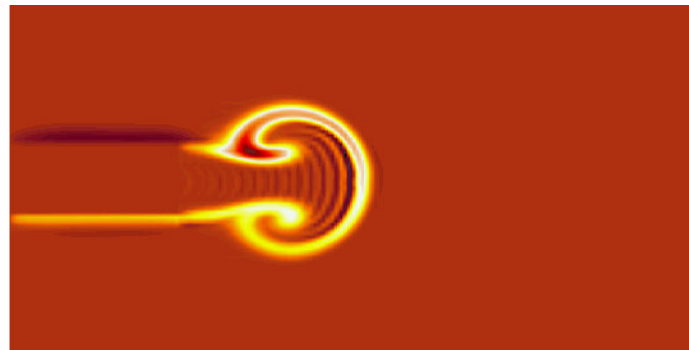


Fig 5 Product (C_p) formation region for turbine model after 0.1s

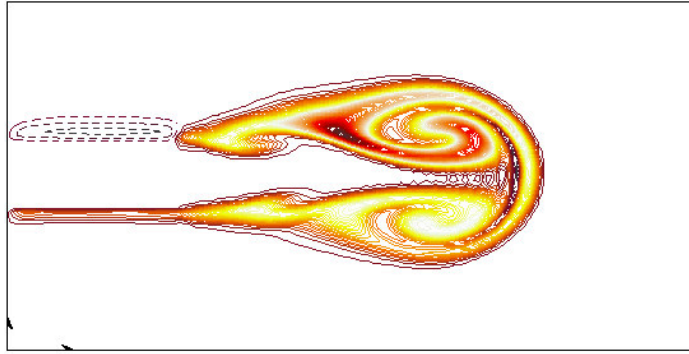


Fig. 6 Product (C_p) formation for turbine model after 1s

Fig. 7 and 8 show the vector field for turbine model. For high Damköhler, $D_a \gg 1$, the flame front is thin compared to the turbulent eddies and its structure is not affected by turbulent fluctuations; such occurs at a flamelet regime (with $K_a < 1$). Turbulence and combustion interacts weakly allowing simplified analysis.

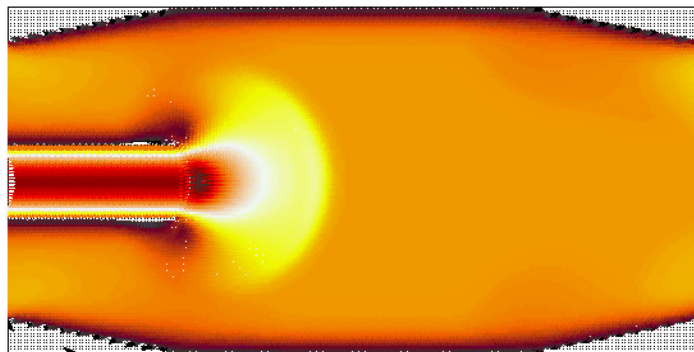


Fig. 7 Vector field for turbine model after 0.1s

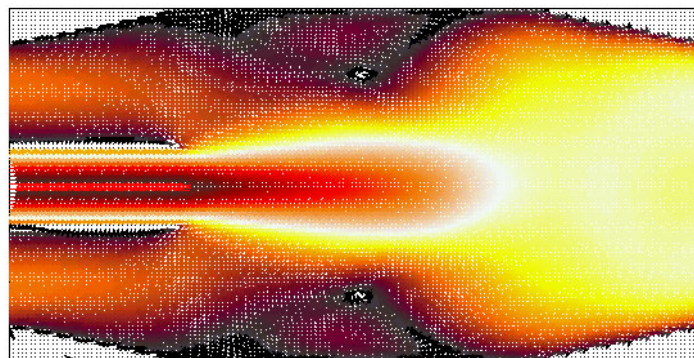


Fig 8. Vector field for turbine model after 1s

Observe the reaction region inside the turbine model after 1 second; this region grows mainly backward the fuel injector. There are indications, for higher time, Damköhler, heat release and Reynolds of the formation of many vortices and a potentially source of disturbance due to the motion and development of these vortices.

5. Conclusions

A computational model is presented for coupling fluid dynamics, chemistry and heat transfer. Computations are performed to obtain a physical understanding of the mixture/reaction global (for coarse meshes) behavior. Consistent results, for reactant and product concentration field, as well as for temperature of reaction are obtained, showing that the model is able to follow non linear behavior of the mixing and reacting progress, for Zel'dovich 10, Damköhler 300 and heat release 10, which are reasonable values for gaseous hydrocarbon chemistry. Results show that for high Damköhler and $K_a < 1$ the flame front is not affected by turbulent fluctuations, permitting a simplified analysis.

It is the author opinion that the finite differences with a proper discretization is useful to obtain a suitable (fast, accurate, simple and cheap) method for the solution of complex flows without introducing many complications to the

conventional code structure. Besides, to develop a working model for solving mixing and reacting flows is not a trivial task; the contribution of this work goes in this direction.

6. Acknowledgement

The present work is being developed under the sponsorship of CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico - Brasil).

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