Direct numerical simulations of high speed reactive mixing layers

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Abstract. The present work is devoted to the analysis of ignition phenomena in high speed turbulent reactive flows. From the computational modelling point of view, this requires to account accurately for the competition between molecular diffusion effects and chemical kinetics as well as complex flowfield structures that may feature shock and expansion waves. Some results of direct numerical simulations of the multicomponent, compressible, reactive Navier-Stokes equations are reported here for the particular case of a two-dimensional mixing layer. Special emphasis is placed on the effects associated with heat release.

1. Introduction
The reduction in the growth rate of mixing layers when the convective Mach number increases is still not fully understood. In reactive mixing layers, it is known from experiments and numerical simulations that heat release due to combustion has similar effects. However, the literature treating both mechanisms, i.e. chemistry-induced heat release and compressibility, simultaneously, is restricted to a few examples, one being the experimental study conducted in [8]. A better understanding of the related phenomena is thus required for applications such as scramjet engines, the efficiency of which depends crucially on a proper mixing of oxidizer and fuel [9]. The objective of the present work is to contribute to the investigation of the conjugated effects of compressibility and combustion in a two-stream mixing layer geometry. The analysis is conducted in the light of DNS results.

2. Description of the numerical solver
2.1. Governing equations
The unsteady, three-dimensional, compressible Navier-Stokes equations are considered for a multi-species reactive gas mixture:

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

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j}, \quad i \in [1,3],
\]

\[
\frac{\partial \rho e_t}{\partial t} + \frac{\partial (\rho e_t + p) u_j}{\partial x_j} = \frac{\partial u_i \tau_{ij}}{\partial x_j} - \frac{\partial q_j}{\partial x_j},
\]

\[
\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho Y_\alpha u_j}{\partial x_j} = - \frac{\partial \rho Y_\alpha V_{\alpha j}}{\partial x_j} + \rho \omega_\alpha, \quad \alpha \in [1,N_{sp}],
\]

where \( \tau_{ij} = 2 \mu (S_{ij} - \delta_{ij} S_{kk}/3) \) and \( S_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2 \). \( \rho e_t = \rho u_i u_i/2 + \rho \sum_{\alpha=1}^{N_{sp}} h_\alpha Y_\alpha - p \) and \( h_\alpha (T_1) = \Delta h_{f\alpha} + \int_{T_0}^{T_1} c_{pe\alpha} (T) dT \). The pressure of the mixture is
given by $p = \rho RT/W$, with $W^{-1} = \sum_{\alpha=1}^{N_{sp}} Y_\alpha/W_\alpha$. $q_j = -\lambda \partial T/\partial x_j + \rho \sum_{\alpha=1}^{N_{sp}} h_\alpha Y_\alpha V_{\alpha j}$ and $Y_\alpha V_{\alpha j} = Y_\alpha \sum_{\beta=1}^{N_{sp}} D_\beta (W_\beta/W) \partial X_\beta/\partial x_j - D_\alpha (W_\alpha/W) \partial X_\alpha/\partial x_j$.

This system of conservative equations is based on the following set of independent variables: the density $\rho$, the momentum $\rho u_i$, the mass fraction of the $N_{sp}$ species $\rho Y_\alpha$ and the total energy $\rho e_t$. Each species behaves as a thermally perfect gas with its thermodynamic properties determined from the JANAF databases [15]. The viscosity $\mu$ and thermal conductivity $\lambda$ depend on the temperature of the mixture as well as its composition. The mixture diffusion coefficients $D_\alpha$ depend on the temperature and pressure of the mixture but the Dufour and Soret effects are not taken into account. The mass production terms $\dot{\omega}_\alpha$ are derived from a set of chemical reaction equations which are expressed in terms of an Arrhenius temperature dependence form, making possible the use of detailed chemical kinetic mechanisms.

2.2. Numerical scheme

The numerical methodology relies on an extension of the numerical solver previously developed by Shahab et al. [12]. The inviscid component of the transport equations is integrated using a seventh-order accurate Weighted Essentially Non-Oscillatory scheme (WENO7) [1, 13] while an eighth-order accurate centered difference scheme is retained for the molecular terms. The time advancement is performed with a third-order accurate TVD low-storage Runge-Kutta scheme [5]. The reactive terms constitute a stiff system of ordinary differential equations which is advanced in time using the DVODE package from CHEMKIN II library [7]. At each time step, the Strang’s splitting technique is adopted following the procedures described in [4, 18].

3. Numerical verification

Preliminary numerical simulations have been performed to assess the performance of the computational solver in simple configurations: original Sod’s shock tube, convergence study, multi-species inert shock tube, diffusion test, perfectly stirred reactor, multi-species reactive shock tube and a laminar premixed flame. In this section we present the two most representative test cases.

3.1. Multi-species reactive shock tube

This problem is a variation of the popular Sod shock tube benchmark applied to a reactive mixture of perfect gases that has been first proposed in [3, 4]. Consider a shock hitting a solid wall boundary and reflecting off. After a delay, a reaction wave kicks in at the boundary, picks up steam and merges with the shock. This test is aimed at validating the correct representation of the competition between the convection and reaction terms, as well as assessing the robustness of the numerical schemes in the presence of strong discontinuities. The one-dimensional Euler equations applied to a reactive gas mixture are solved. The mixture under consideration is characterized by a $2/1/7$ molar ratio of $H_2/O_2/Ar$. The initial conditions correspond to the following Riemann problem: $(\rho_L, u_L, P_L) = (0.072 \text{ kg/m}^3, 0 \text{ m/s}, 7173 \text{ Pa})$, $(\rho_R, u_R, P_R) = (0.18075 \text{ kg/m}^3, -487.34 \text{ m/s}, 35594 \text{ Pa})$. The left (L) and right (R) sides are separated by a membrane that is placed at the middle of a 12 cm domain discretized with 400 grid points. Wall boundary condition is set at $x = 0 \text{ cm}$ and perfectly non-reflecting at $x = 12 \text{ cm}$. The value of the convective CFL number is set to 0.5. Finally, the detailed chemical kinetic mechanism is reported in Table 3.
Figure 1. Shock tube with a H\textsubscript{2}/O\textsubscript{2}/Ar mixture and a discontinuity initially placed at \(x = 6 \text{ cm}\). Profiles of temperature (a), velocity (b), ratio of specific heats (c) and mass fraction of H (d). 400 grid points, \(CFL = 0.5\).

Figure 1 displays some numerical results at three different times. At \(t = 170 \mu\text{s}\) the reactive wave has not yet reached the reflected shock. The results corresponding to the state obtained after the shock reflection are very similar to those reported in [3, 4]. However, in comparison with [3, 4], the reactive wave moves faster in the present calculation which can be ascribed to the different kinetic schemes used in [3, 4].

3.2. One-dimensional hydrogen/oxygen laminar premixed flame

This benchmark test aims at assessing the numerical solver in situations where the orders of magnitude of the convection, diffusion and reactive contributions are similar. We study the combustion of an hydrogen-oxygen mixture using the reaction mechanism of Eklund (see Table 4). Following the strategy retained in [18], we compare the solution obtained using the numerical solver with a reference solution. The reference solution is obtained with the PREMIX package [6] from the CHEMKIN library for a lean mixture, the equivalence ratio is set to \(\phi = 0.8\). The temperature and pressure in fresh reactants are, respectively, 298 K and 1 atm. The three
centimeters long computational domain is discretized by using 2000 grid points. Our CFD final solution is obtained using PREMIX reference solution as the initial condition with compatible boundary conditions: Dirichlet boundary conditions are fixed at the inflow where the values of temperature, pressure, composition and velocity are set; at the outflow boundary, the gradients of mass fractions and temperature are set to zero while the pressure is held constant. The Navier-Stokes simulation is conducted with a convective CFL number value of 0.7 until a physical time of 1 ms.

Figure 2 illustrates the excellent agreement obtained between the present numerical solutions and the reference solutions given by PREMIX. All the variables are plotted in S.I. units as a function of the progress variable of the chemical reaction, defined by 

\[ c = \frac{(T - T_u)}{(T_b - T_u)} \]

where \( T_u \) is the temperature in the fresh reactants and \( T_b \) is the temperature in the fully burned gases.

**Figure 2.** One-dimensional hydrogen-oxygen laminar premixed flame. Comparison between solutions obtained with PREMIX (CHEMKIN library) and the present multi-species reactive Navier-Stokes numerical simulation at \( t = 1 \text{ ms} \). Variables are plotted as a function of the progress variable \( c = (T - T_u)/(T_b - T_u) \). 2000 grid points, \( CFL = 0.7 \). S.I. units.

4. Two-dimensional supersonic reactive mixing layers

This problem is set into a two-dimensional Cartesian coordinate system. The computational domain has a length \( L_x \) along \( x \) and \( L_y \) along \( y \). The top section (1) is the fuel region and the bottom (2), air. The flow is initialized using a hyperbolic tangent profile for the streamwise velocity component, while the other component is set to zero:

\[ u(y) = \frac{1}{2} \left[ (U_1 + U_2) + (U_1 - U_2) \tanh \left( \frac{y}{2\delta_0} \right) \right], \quad v = 0. \quad (5) \]

The mass fraction profiles are initialized according to:

\[ Y_\alpha(y) = Y_{\alpha 0} \left[ 1 + \lambda_\alpha(s) \tanh \left( \frac{y}{2\delta_0} \right) \right], \quad (6) \]

where \( \lambda_\alpha(s) = (Y_{\alpha 2}/Y_{\alpha 1} - 1)/(Y_{\alpha 2}/Y_{\alpha 1} + 1) \) and \( Y_{\alpha 0} = (Y_{\alpha 1} + Y_{\alpha 2})/2 \).
Table 1. Parameters of the supersonic mixing layer.

| Quantity            | Fuel stream | Oxidizer stream |
|---------------------|-------------|-----------------|
| Pressure (Pa)       | 101325.0    | 101325.0        |
| Temperature (K)     | 2000.0      | 2000.0          |
| Velocity (m/s)      | 2670.0      | 1814.0          |
| $Y_{H_2}$ (--)      | 0.1         | 0.0             |
| $Y_{O_2}$ (--)      | 0.0         | 0.232           |
| $Y_{N_2}$ (--)      | 0.9         | 0.768           |

Table 1 provides the other parameters relevant to the present simulation. The results discussed below correspond to a convective Mach number $M_c = 0.38$. The Reynolds number $Re_\theta$, based on the initial momentum thickness $\delta^0_\theta$ and $\Delta U = U_1 - U_2$, is set to 160, which corresponds to a value of $\delta^0_\theta = 9.35 \times 10^{-5}$ m. The domain size, non-dimensionalized by $\delta^0_\theta$, is given by $L^*_x \times L^*_y = 350 \times 120$ with $N_x \times N_y = 875 \times 200$ grid points. The reaction model chosen corresponds to a global single step reaction (see table 5). Perfectly non-reflecting boundary conditions are imposed at the bottom, top and outflow boundaries while fluctuating Dirichlet boundary conditions are applied at the inflow to trigger the development of the shear layer. To ensure the stability of the numerical simulations, the value of the convective CFL number is set to 0.7, the Fourier number $F_0$ is set to 0.1, and the time step is restricted to a combustion-induced increase of temperature of $\Delta T = 50$ K.

Figure 3. Two-dimensional supersonic mixing layer. Spatial evolution of the vorticity thickness (a) and the momentum thickness (b) for both inert and reactive cases.

Figure 3 shows the evolution along the $x$-direction of the non-dimensional vorticity and momentum thicknesses of the mixing layer for both inert and reactive cases. These quantities are defined, respectively, as $\delta_\omega(x) = \Delta U/(\bar{\partial u}/\partial y)_{\text{max}}$ and $\delta_\theta(x) = \int_{-L_y/2}^{L_y/2} (\bar{\rho}(\bar{u} - U_2)(U_1 - \bar{u})/(\rho_\infty \Delta U^2)) dy$, where $\bar{\rho}$ denotes the Reynolds averaged value of the density and $\bar{u}$ denotes the Favre averaged value of the streamwise velocity.
Table 2. Comparison of some typical results for several configurations of inert mixing layers obtained by different authors.

| $Re_\theta$ | $\sigma_{uu,max}$ | $\sigma_{vv,max}$ | $\sigma_{uv,max}$ | $K_\delta$ | Type       | Reference                                |
|-----------|------------------|-------------------|------------------|-----------|-----------|------------------------------------------|
| -         | 0.176            | 0.138             | 0.097            | 0.190     | Experimental | Wygnanski & Fiedler [17] |
| 450       | 0.180            | 0.140             | 0.100            | 0.163     | DNS-3D     | Bell & Mehta [2]                      |
| 800       | 0.160            | 0.130             | 0.100            | 0.130     | DNS-3D     | Rogers & Moser [10]                    |
| 90        | 0.200            | 0.200             | 0.150            | 0.143     | DNS-2D     | Stanley & Sarkar [16]                  |
| 160       | 0.230            | 0.280             | 0.110            | 0.164     | DNS-2D     | Present simulation                     |

**Figure 4.** Two-dimensional supersonic shear layer. Profiles of the mean streamwise velocity (a) and turbulent shear stresses (b)-(d) as a function of $y/\delta_\omega(x)$. Results are shown at $x = 220\delta_\omega$, $x = 270\delta_\omega$ and $x = 320\delta_\omega$ for the inert (I) and reactive (R) cases.

The vorticity thickness yields a linear growth, that is $d\delta_\omega/dx = K_\delta(U_1 - U_2)/(U_1 + U_2)$. For the inert case, a value of $K_\delta = 0.164$ is found, which is in good agreement with experimental data and numerical simulations from various authors as shown in Table 2. For the reactive case, the effect of heat release is found to decrease significantly the value of $K_\delta$. This confirms the
early observations of Sekar and Mukunda [11]. A value of $K_3 = 0.075$ is found, which is however significantly lower than the one predicted by these authors. Figure 4 illustrates the profiles of mean streamwise velocity and the turbulent shear stresses $\sigma_{uu} = \sqrt{\bar{u}''^2/\Delta U}$, $\sigma_{vv} = \sqrt{\bar{v}''^2/\Delta U}$ and $\sigma_{uv} = \sqrt{\bar{u}''\bar{v}''/\Delta U}$, as a function of $y/\delta_u(x)$ at three different locations: $x = 220\delta_u^0$, $x = 270\delta_u^0$ and $x = 320\delta_u^0$. The self-similarity of the mean streamwise velocity profiles is well reproduced along the three different positions for both inert and reactive cases. As expected, the values obtained for the inert case confirm that the shear stresses are in fact overestimated in the present 2D simulation in comparison with experimental data or 3D DNS simulations. Two dimensional numerical simulations indeed refrains the action of turbulent mixing, and leads to overestimated levels the turbulent energy. Nevertheless, the present values are similar to those obtained by Stanley and Sarkar in their two-dimensional DNS. The present results thus confirm that the heat release reduces the turbulent shear stresses in the reactive case, which is in agreement with the conclusion previously given in [11].

5. Summary
Some direct numerical simulations of inert and reactive two-dimensional compressible mixing layers have been performed. It is found that the effects of heat release influences the spatial development of mixing layers in a globally similar fashion as compressibility effects. The momentum thickness growth rates and Reynolds shear stresses are reduced when exothermic chemical reactions set in. Three-dimensional direct numerical simulations including detailed chemistry are now in progress to (i) confirm these trends, (ii) further elaborate the analysis of mixing efficiency by considering both the large and small scale mixing characteristics.

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Reaction rate constants for the mechanism of Kee et al. [6]. Reaction coefficients are written in the form $k_f = AT^\beta \exp(-E_0/R_0T)$ in s-cm$^3$-cal-mol-K. The species considered are: H$_2$, O$_2$, H, O, OH, HO$_2$, H$_2$O$_2$, H$_2$O, Ar.

Table 3. Reaction rate constants for the mechanism of Kee et al. [6]. Reaction coefficients are written in the form $k_f = AT^\beta \exp(-E_0/R_0T)$ in s-cm$^3$-cal-mol-K. The species considered are: H$_2$, O$_2$, H, O, OH, HO$_2$, H$_2$O$_2$, H$_2$O, Ar.

| N | Reaction                  | A       | $\beta$ | $E_0$   |
|---|---------------------------|---------|---------|---------|
| 1 | H$_2$ + O$_2$ = 2OH       | 1.70 \times 10^{13} | 0.00    | 47780   |
| 2 | OH + H$_2$ = H$_2$O + H   | 1.17 \times 10^9  | 1.30    | 3626    |
| 3 | H + O$_2$ = OH + O        | 5.13 \times 10^{16} | -0.816 | 16507   |
| 4 | O + H$_2$ = OH + H        | 1.80 \times 10^{10} | 1.00   | 8826    |
| 5 | H + O$_2$ + M = HO$_2$ + M$^a$ | 2.10 \times 10^{18} | -1.00  | 0       |
| 6 | H + 2O$_2$ = HO$_2$ + O$_2$ | 6.70 \times 10^{19} | -1.42  | 0       |
| 7 | OH + HO$_2$ = H$_2$O + O$_2$ | 5.00 \times 10^{13} | 0.00   | 10000   |
| 8 | H + HO$_2$ = 2OH          | 2.50 \times 10^{14} | 0.00   | 1900    |
| 9 | O + HO$_2$ = O$_2$ + OH   | 4.80 \times 10^{13} | 0.00   | 10000   |
|10 | 2OH = O + H$_2$O          | 6.00 \times 10^{8}   | 1.30   | 0       |
|11 | H$_2$ + M = 2H + M$^b$    | 2.25 \times 10^{12} | 0.50   | 92600   |
|12 | O$_2$ + M = 2O + M        | 1.85 \times 10^{11} | 0.50   | 95560   |
|13 | H + OH + M = H$_2$O + M$^c$ | 7.50 \times 10^{23} | -2.00  | 0       |
|14 | H + HO$_2$ = H$_2$O + O$_2$ | 2.50 \times 10^{13} | 0.00   | 700     |
|15 | 2HO$_2$ + = HO$_2$ + O$_2$ | 2.00 \times 10^{12} | 0.00   | 0       |
|16 | H$_2$O$_2$ + M = 2OH + M  | 1.30 \times 10^{17} | 0.00   | 45500   |
|17 | H$_2$O$_2$ + H = HO$_2$ + H$_2$ | 1.60 \times 10^{12} | 0.00   | 3800    |
|18 | H$_2$O$_2$ + OH = H$_2$O + HO$_2$ | 1.00 \times 10^{13} | 0.00   | 1800    |

$^a$Third body efficiency: $k$(H$_2$O) = 21, $k$(H$_2$) = 3.3.

$^b$Third body efficiency: $k$(H$_2$O) = 6, $k$(H) = 2, $k$(H$_2$) = 3.

$^c$Third body efficiency: $k$(H$_2$O) = 20.

Table 4. Reaction rate constants for the mechanism of Eklund. Reaction rate coefficients are written in the form $k_f = AT^\beta \exp(-E_0/R_0T)$ in s-cm$^3$-cal-mol-K. The species considered are: H$_2$, O$_2$, H, O, OH, H$_2$O.

| N | Reaction                  | A       | $\beta$ | $E_0$   |
|---|---------------------------|---------|---------|---------|
| 1 | H$_2$ + O$_2$ = 2OH       | 0.170 \times 10^{14} | 0.00    | 48150   |
| 2 | H + O$_2$ = O + OH        | 0.142 \times 10^{15} | 0.00    | 16400   |
| 3 | OH + H$_2$ = H$_2$O + H   | 0.316 \times 10^{8}   | 1.80   | 3030    |
| 4 | O + H$_2$ = OH + H        | 0.207 \times 10^{15} | 0.00    | 13750   |
| 5 | 2OH = O + H$_2$O          | 0.550 \times 10^{14} | 0.00    | 7000    |
| 6 | H + OH + M = H$_2$O + M   | 0.221 \times 10^{23} | -2.00  | 0       |
| 7 | 2H + M = H$_2$ + M        | 0.653 \times 10^{18} | -1.00  | 0       |

Table 5. Reaction mechanism retained for the supersonic mixing layer simulation. Reaction rate coefficients are written in the form $k_f = AT^\beta \exp(-E_0/R_0T)$ in s-cm$^3$-cal-mol-K. The species considered are: H$_2$, O$_2$, H$_2$O, N$_2$.

| N | Reaction                  | A       | $\beta$ | $E_0$   |
|---|---------------------------|---------|---------|---------|
| 1 | 2H$_2$ + O$_2$ = 2H$_2$O   | 1.10 \times 10^{19} | 0.00    | 16077   |