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Ignition and Flame Studies for Turbulent Transonic Mixing in a Curved Duct Flow

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A computational method is developed for solving the full compressible Navier-Stokes equations with multiple species and chemical reactions. The code is used to study a two-dimensional diffusion flame in a transonic flow with large pressure gradients typical of conditions in a turbine passage. The effect of turbulence is considered by using the Baldwin-Lomax algebraic turbulence model. The numerical solutions are used to study the flame structure in a transonic flow under the influence of large axial and transverse pressure gradients. Solutions in a straight duct with only streamwise pressure gradient are compared with those in curved ducts with both streamwise and transverse pressure gradients.

Nomenclature

- $C_p$: specific heat
- $D$: diffusivity
- $E$: stagnation energy
- $f$, $g$: Euler flux vectors
- $f_i$, $g_i$: Navier-Stokes flux vectors
- $h$: enthalpy
- $h^0$: heat of formation
- $h^0$: heat of formation
- $M$: Mach number
- $N$: total number of species
- $p$: pressure
- $Pr_L$: laminar Prandtl number
- $Pr_T$: turbulent Prandtl number
- $\dot{Q}$: heat production due to reaction
- $R$: gas constant number based on length $s$
- $Re_x$: Reynolds number based on length $x$
- $T$: temperature, K
- $u$: velocity in $x$ or $s$ direction
- $v$: velocity in $y$ direction
- $V$: velocity
- $V_d$: diffusion velocity
- $W$: molecular weight
- $x$, $y$: cartesian coordinates
- $Y$: mass fraction
- $\bar{Y} = \int \rho u Y dy / \int \rho dy$, cross-sectional average

Greek symbols

- $\mu$: molecular viscosity
- $\mu_T$: turbulent viscosity

Subscripts

- $i$: species $i$
- $ij$: tensor subscript for $x$ and $y$
- $ref$: reference values
- $\infty$: freestream
- $0$: inlet

Introduction

Designers of jet engines are attempting to increase the thrust-to-weight ratio and to widen the range of engine operation. Since the flow in a turbine passage is accelerating and power is extracted from the flow, it is possible to add heat without increasing the flow temperature beyond the turbine blade material limit. Sirignano and Liu\cite{1,2} show by thermodynamic analysis that the thrust of aircraft turbojet and turbofan engines can be increased significantly with little increase in fuel consumption by intentionally burning fuel in the turbine stages. For the ground-based gas turbine, benefits have been shown to occur in power/weight and efficiencies.\cite{1} A mixing and exothermic chemical reaction in the accelerating flow through the turbine passage offers, therefore, an opportunity for a major technological improvement. The gas turbine engine is not the only potential application for this technology. The reduction in peak temperatures due to acceleration results in the promise of reduced pollutant formation and reduced heat transfer losses in many other combustion applications.

In order to provide insight into the fundamental behavior of multidimensional flows with mixing and
chemical reaction in the presence of strong pressure gradients that support a transonic flow, Sirignano and Kim\(^3\) obtained similarity solutions for laminar, two-dimensional, mixing, reacting and nonreacting layers with a pressure gradient that accelerates the flow in the direction of the primary stream. Fang, Liu and Sirignano\(^4\) extended that study to mixing layers with arbitrary pressure gradients by using a finite difference method for the boundary layer equations. The influence of pressure gradient, initial temperature, initial pressure, initial velocity, and transport properties were studied. These solutions offer insight into the passage. However, they are restricted to only laminar flows and do not account for the transverse pressure gradient that are typical in a turbine blade passage.

Mehring, Liu, and Sirignano\(^5\) extends the laminar boundary layer calculations of Fang, Liu, and Sirignano\(^4\) to include turbulence. In this paper, we develop a finite-volume method for solving the two-dimensional full compressible Navier-Stokes equations with chemical reaction without the assumption of a thin mixing layer. Turbulence is included by using the Baldwin-Lomax turbulence model. Computational results are first compared with solutions obtained in the laminar mixing layer studies using the boundary layer method by Fang, Liu and Sirignano.\(^4\) The method is then extended to treat transonic turbulent mixing flows in a curved duct to examine the ignition and combustion processes in a general transonic accelerating mixing layer.

**Governing Equations and the Computational Method**

The flow within a turbine blade row is at high speed and often transonic. There are large gradients of pressure, density and velocity in the flow field. One needs to investigate the mutual interaction between the combustion processes and the flow to understand both the combustion and determine the aerodynamic performance of the turbine blade rows. For this purpose, a model that is capable of handling transonic flow and chemical reaction is needed.

A finite-volume method with multigrid for accurately calculating the flow through turbomachinery blade rows based on the above system of equations was developed by Liu and Zheng.\(^6,7\) A flux-difference splitting scheme based on Roe splitting has also been developed.\(^8\) Although there has been much work on computation of reactive flows, there are practically none on high speed reacting flows in turbomachines. In this research we extend our CFD code for turbomachinery flows to include appropriate chemical reaction models.

The two-dimensional, Favre-averaged Navier-Stokes equations for \(N\) species are written in integral form over a fixed control volume \(\Omega\)

\[
\frac{\partial}{\partial t} \int_{\Omega} \theta(x,y) w \, d\Omega + \oint_{\partial \Omega} \theta(x,y) (f \, dS_x + g \, dS_y) = \oint_{\partial \Omega} \theta(x,y) s \, d\Omega \quad (1)
\]

where the vector \(w\) is formed by the conservative variables for mass, momentum, energy, \(f\) and \(g\) are the convective flux vectors; \(f_\mu\) and \(g_\mu\) are the diffusive flux vectors; and \(S\) is a volume source term. These are given as

\[
w = \begin{pmatrix} \rho_i \\ \rho u_i \\ \rho v_i \\ \rho E_i \end{pmatrix}, \quad s = \begin{pmatrix} \frac{\dot{\omega}_i}{\rho} \\ \frac{\partial p_i}{\partial x_i} + \frac{\rho u_i v_i}{\rho} \\ \frac{\partial p_i}{\partial y_i} + \frac{\rho v_i u_i}{\rho} \\ \frac{\partial p_i}{\partial z_i} \end{pmatrix}
\]

\[
f = \begin{pmatrix} \rho_i u_i \\ \rho u_i v_i + p \\ \rho u_i u_i \\ \rho u_i v_i + p \end{pmatrix}, \quad g = \begin{pmatrix} \rho v_i \\ \rho u_i v_i + p \\ \rho v_i v_i + p \\ \rho v_i u_i + p \end{pmatrix}
\]

\[
f_\mu = \begin{pmatrix} -\rho_i u_i d_i \\ \tau_{xx} \\ \tau_{yx} \\ \tau_{yy} \end{pmatrix}, \quad g_\mu = \begin{pmatrix} \rho_i v_i d_i \\ \tau_{xy} \\ \tau_{yy} \end{pmatrix}
\]

In the above equations \(t\) is time, \(\rho_i\) density for species \(i\), \(p\) pressure, \(\mu\) molecular viscosity; \(u\) and \(v\) are the flow velocity components in the \(x\) and \(y\) directions, respectively. The streamtube thickness function \(\theta(x)\) is equivalently the channel height in the third dimension in order to vary the cross-sectional area of a channel with constant width so that a streamwise pressure gradient may be imposed on the flow. Other quantities are defined in the following equations:

\[
\tau_{ij} = 2(\mu + \mu_T) \left[ \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] (6)
\]

\[
q_j = -C_p \left( \frac{\mu}{Pr_L} + \frac{\mu_T}{Pr_T} \right) \frac{\partial T}{\partial x_j} (7)
\]

\[
h = \sum_{i=1}^{n} Y_i h_{i,i}, \quad \text{and} \quad h_i = \int_{T_0}^{T} C_{pi} dT (8)
\]

\[
\dot{Q} = \sum_{i=1}^{N} \dot{\omega}_i h_{i,0} (9)
\]

where \(h_{i,0}^0\) is the heat of formation of species \(i\) at the reference temperature \(T_0\). \(C_{pi}\) is the specific heat capacity of species \(i\).
A perfect gas is assumed

\[ p = \sum_{i=1}^{N} \rho_i R_i T \]  \hspace{1cm} (10)

\[ \rho = \sum_{i=1}^{N} \rho_i \]  \hspace{1cm} (11)

\[ H = h + \frac{1}{2}(u^2 + v^2) \]  \hspace{1cm} (12)

\[ E = H - \frac{p}{\rho} \]  \hspace{1cm} (13)

\[ \rho_i \nabla v_i = -\rho D_i \nabla \left( \frac{\rho_i}{\rho} \right) \]  \hspace{1cm} (14)

Methane (CH₄) is used for the current computations although the method is not restricted to only one type of fuel. The combustion process is described by the same one-step overall chemical reaction used in Ref. 4 as:

\[ CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2 \]

The chemical kinetics rate for the fuel is:

\[ \omega_F = W_F A e^{-E_a/RT} [Fuel]^a [O_2]^b \]  \hspace{1cm} (15)

where the brackets \([ \ ]\) represent molar concentration in mol/cm³. According to Ref. 9, for methane (CH₄), A = 2.8×10⁹ 1/second, E_a = 48.4 kcal/mol, a = -0.3, b = 1.3.

In the solution procedure, the average gas constant \(R\), molecular weight \(W\), viscosity coefficient \(\mu\) can be obtained by the following equations:

\[ R = \sum_{i=1}^{N} R_i Y_i \]  \hspace{1cm} (16)

\[ \frac{1}{W} = \sum_{i=1}^{N} \frac{1}{W_i} Y_i \]  \hspace{1cm} (17)

\[ \mu = \sum_{i=1}^{N} \mu_i(T)Y_i. \]  \hspace{1cm} (18)

The molecular viscosity coefficient of each species \(\mu_i\) is obtained by using Sutherland-law:

\[ \frac{\mu_i}{\mu_0} = \left( \frac{T_i}{T_0} \right)^{\frac{3}{2}} \frac{T_0 + 110}{T + 110} \]  \hspace{1cm} (19)

The turbulent viscosity \(\mu_T\) is determined by the Baldwin-Lomax algebraic turbulence model:

\[ \mu_t = KC_{cp} \rho F_{wake} F_{kleb}(y) \]  \hspace{1cm} (20)

\[ F_{wake} = \min(y_{max}, F_{max}, C_{wk} y_{max} U_{diff}^2 / F_{max}) \]  \hspace{1cm} (21)

\[ F(y) = y \left[ \frac{1}{2} \left( \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \right] \]  \hspace{1cm} (22)

Notice that the species equation has the same form as the basic conservation equations. Consequently, the same numerical method for the Navier-Stokes equations can be readily applied to the species conservation equations. An implicit algorithm for solving source terms is implemented in our method for solving the turbulence model equations. The same technique is extended to treat chemical reaction terms to avoid the stiffness introduced by the source terms of the reactions. The total continuity equation is used as a check to the global mass conservation.

**Computational Results**

**Laminar Flow in a Straight Shear Layer**

Consider a diffusion flame in the two-dimensional, laminar, steady, viscous, multicomponent, compressible mixing layer in the presence of a pressure gradient. At the trailing edge of a flat splitter plate \((x = 0)\), the hot air mixed with burned gases flowing above the flat plate at the velocity \(u_{\infty}\) comes into contact with a fuel vapor flowing below the flat plate at the velocity \(u_{-\infty}\). Then, a chemical reaction takes place between the air and the fuel vapor, and a diffusion flame will be established near the middle of the shear layer. Ref. 4 studied by solving the boundary layer equations the laminar flame structure of the above problem under 13 different flow conditions. One of these cases is identified as the Base Case, which corresponds to a streamwise pressure gradient of \(-200 \text{ atm}/\text{m}\). The initial total pressure of the gases are at 30 atm. The initial velocity and temperature of the air are \(u_{air} = 50 \text{ m/s}\) and \(T_{air} = 1600 \text{ K}\), respectively, and those of the fuel (methane) are \(u_F = 25 \text{ m/s}\) and \(T_F = 400 \text{ K}\). In this section, this Base Case is used to validate the present full Navier-Stokes code.

Figures 1, 2, and 3 compare the velocity, temperature, and density profiles at \(x = 5 \text{ cm}\) and 7.5 cm downstream of the trailing edge of the splitter plate as obtained by the present method and the boundary layer method in Ref. 4. It is noticed that the full Navier-Stokes solution agrees with the boundary solutions in general. However, the full Navier-Stokes solution is more diffusive, resulting in thicker velocity, temperature and density shear layers. This is perhaps due to the existence of numerical diffusion present in the solutions. The greater diffusion causes the a higher maximum flame temperature in the middle of the shear layer as shown by Figure 2. This, in turn, results in a lower density, and consequently a higher velocity shown in Figures 1 and 3.

Figure 4 shows the mass fraction distributions for oxygen, methane, and the combustion product at \(x = \)
Turbulent Flow in a Straight Shear Layer

Once the code is validated for laminar flow, it is extended to calculate turbulent flow for the same base case as above. The Reynolds number for this flow is 172810/cm based on the inlet flow conditions. The Baldwin-Lomax algebraic model is used in regions where \( \text{Re}_x \geq 10^6 \).

Figures 5, 6, and 7 show the velocity, temperature and density profiles at the three locations that correspond to pressure ratios of \( p/p_0 = 0.75 \), \( 0.60 \), and \( 0.45 \), where \( p_0 \) is the pressure at \( x = 0 \). The turbulent solutions are almost one order of magnitude thicker than the laminar solutions. However, the basic behavior of the solutions remain the same. It is noticed that the maximum temperature of the turbulent flame is a little higher than the laminar flame, and the location is also different from that of the laminar flame. The flame tends to move towards the air side because of the increased combustion rate.

Figure 8 shows the mass fraction distributions for oxygen, methane, and the combustion product at \( p/p_0 = 0.45 \). The profile for the product mass fraction is significantly wider, indicating that there is a lot more fuel being consumed due to the increased combustion rate under turbulent conditions.
Fig. 6 Temperature profiles at three streamwise locations downstream of the trailing edge of the splitter plate, turbulent base case.

Fig. 7 Density profiles at three streamwise locations downstream of the trailing edge of the splitter plate, turbulent base case.

Fig. 8 Mass fraction profiles at $p/p_0 = 0.45$ location downstream of the trailing edge of the splitter plate, turbulent base case.

Fig. 9 Schematic of two curved channel and a straight channel.

Mixing Layer in a Curved Duct

In order to simulate the flow conditions in a typical HP turbine passage, a curved channel with fuel/air mixing is considered. Three different cases shown in Figure 9 are studied and compared to each other. In all three cases, the top half of the channel is injected with hot air at the inlet, while the bottom half is injected with fuel. Channel 1 is the base straight channel case. Channel 2 curves upward with a radius of $R = 0.5099$. Channel 3 curves downward with a radius of $R = 0.3183$. The streamwise pressure gradients are kept the same for all three cases by appropriately adjusting the streamtube thickness function $\theta(s)$. All other conditions are kept the same as the base case. Inviscid boundary conditions are used on the channel walls since the focus of the study is the effect of transverse pressure gradient on the flame. Figures 10, 11, and 12 are the computed pressure contours for the three cases. There is no transverse pressure gradient in the straight channel. The flows in Channel 2 and Channel 3 show significant transverse pressure gradient due to flow turning. Channel 3 has a stronger transverse pressure gradient due to its smaller radius of curvature.

Figures 13, 14, and 15 show the velocity, temperature, and density profiles at distances $s = 5$ cm and $s = 7$ cm, where $s$ is the arc-length at the center of the channel measured from the inlet. Despite the large differences in the magnitude and direction of the transverse pressure gradients, the solutions near the center line are essentially unchanged. There are, however, large differences towards either side of the channel walls since there are large differences in the pressure, density, and velocity values in those regions due to the
Fig. 10 Contours of pressure for Channel 1.

Fig. 11 Contours of pressure for Channel 2.

Fig. 12 Contours of pressure for Channel 3.

Fig. 13 Velocity distributions at $s = 5\, cm$ and $s = 7\, cm$.

Fig. 14 Temperature distributions at $s = 5\, cm$ and $s = 7\, cm$.

Fig. 15 Density distributions at $s = 5\, cm$ and $s = 7\, cm$.

transverse pressure gradients. Figure 16 shows the Mach number distribution at the same streamwise locations. It is noticed again that there are little differences among the three solutions near the centerline despite large differences near the channel walls. Notice also that the flows become sub-sonic due to the elevated temperature inside the flame even though they are supersonic outside.

Figures 17 and 18 plot the mass fraction profiles of...
oxygen, fuel, and combustion product at $s = 5 \text{ cm}$ and $s = 7 \text{ cm}$, respectively. This time, the three solutions are almost identical all across the duct. The different pressure values near the channel walls do not affect the species concentrations.

The above results indicate that the flame stays relatively close to the centerline of the channel, where the conditions are the same for the same streamwise pressure gradient despite the wide disparities in transverse pressure gradients. The transverse pressure gradient does not seem to affect the flame structure. In order to further demonstrate this, Figures 19, 20, 21, and 22 plot values of pressure, velocity, temperature, density, and mass fraction of product along the center line of the channel. The three cases show the same distribution at the center of the channels. Figures 19 and 20 show that the pressure decreases while velocity increases along the streamwise direction. The temperature and density variations shown in Figures 21, 22 show clearly the ignition process at about $s = 0.6 \text{ cm}$ when the temperature suddenly rises and the density drops because of the temperature rise. Figure 23 plots the average mass fraction of product $Y_p$ at each cross section along the channels, which is an integrated measure of the total product starting from the inlet. It can be seen that the amount of product shows a sudden increase after ignition and then increases steadily due to continued combustion.

**Fuel Injected in the Middle of a Curved Channel**

Consider the situation where fuel is injected at the inlet between 20% below and 20% above the centerline of the three curved channels discussed in the above section. Figures 24 and 25 shows the velocity and Mach number distributions.
number distributions in the direction normal to the centerline (shown as \( y \) in the figure) at \( s = 5 \, \text{cm} \) and \( s = 7 \, \text{cm} \) where \( s \) is the arclength along the centerline of the channel. Only results for Channels 1 and 3 are shown. There are two peaks along the \( y \) direction which correspond to the two flames where air and fuel are in contact. Figures 26 and 27 are the temperature distributions at \( s = 5 \, \text{cm} \) and \( s = 7 \, \text{cm} \), respectively. Figure 28 plots the density distribution at the same streamwise locations across the channels. The elevated temperature levels in the two flame regions reduce the density of the fluid. Lighter fluid is then accelerated more for the same streamwise pressure gradient, resulting in the velocity peaks. The Mach number in the flames, however, are lower due to the higher local sound speed.

While the Mach number distribution for the straight channel maintains symmetry about the centerline, the Mach number for the curved channel exhibits obvious asymmetry. The Mach number toward the outer wall of the channel is much lower than that near the inner wall. In order to turn the flow in the curved channel, there much be a pressure gradient in the radial direction. The pressure near the outer wall must be greater than that in the inner wall. This is clearly seen in the computed pressure distribution in the \( y \) direction at \( s = 5 \, \text{cm} \) and \( s = 7 \, \text{cm} \) shown in Figure 29. The pressure at \( s = 7 \, \text{cm} \) is smaller than that at \( s = 5 \, \text{cm} \) due to the negative streamwise pressure gradient. The pressure distributions for Channel 1 are constant in the \( y \) direction. The low pressure near the inner wall gives rise to the higher velocity and thus higher Mach number shown in Figures 24 and 25.

It is seen from Figures 26 and 27 that compared to the flames in the straight channel the lower flame (closer to the inner wall) for Channel 3 is thinner while the upper flame is thicker than those for Channel 1. This is also evident in the distributions of fuel, oxygen, and combustion product along \( y \) at \( s = 5 \, \text{cm} \) and \( s = 7 \, \text{cm} \) shown in Figures 30 and 31. The lower velocity in the outer region effectively increases mixing.
Fuel Injection into a Curved Channel Typical of a Turbine Blade Passage

Figure 33 shows the geometric configuration and the computed Mach number distribution in a curved channel typical of a turbine blade passage. The Mach number at the inlet of the duct is close to 0.1. The flow accelerates inside the duct from subsonic to supersonic. The Mach number at the exit of the duct is 1.4. There are large pressure gradients along the flow direction and also normal to the flow direction. Fuel is injected in the middle of this channel at the inlet. Figure 34 plots the temperature contours in the channel. The two flames at the interfaces between fuel and air in the transverse direction, and therefore gives rise to a thicker mixing layer and thus a thicker flame. It is also noticed that the two flames in the curved channel spread wider than those in the straight channel, indicating that the curved wall enhances combustion in a global sense. This is also evidenced by the greater amount of product $Y_p$ produced in the curved channel shown in Figure 32. The temperature in the curved channel is generally higher than that in the straight channel.

Fig. 25 Mach number distribution in Channels 1 and 3 with fuel injected in the middle.

Fig. 26 Temperature distribution in Channels 1 and 3 with fuel injected in the middle at $s = 5\, \text{cm}$.

Fig. 27 Temperature distribution in Channels 1 and 3 with fuel injected in the middle at $s = 7\, \text{cm}$.

Fig. 28 Density distribution in Channels 1 and 3 with fuel injected in the middle at $s = 5\, \text{cm}$ and $s = 7\, \text{cm}$.

Fig. 29 Pressure distribution in Channels 1 and 3 with fuel injected in the middle.
Fig. 30 Mass concentration for fuel, oxygen, and combustion product in Channels 1 and 3 with fuel injected in the middle at $s = 5 \, \text{cm}$.

Fig. 31 Mass concentration for fuel, oxygen, and combustion product in Channels 1 and 3 with fuel injected in the middle at $s = 7 \, \text{cm}$.

Fig. 32 Variation of cross-sectional average of mass fraction of product along the axial direction for Channels 1 and 3.

Fig. 33 Mach number contours in a channel typical of a turbine blade passage.

Fig. 34 Temperature contours in a channel typical of a turbine blade passage. They are clearly seen. The higher temperatures again result in the lower Mach numbers in the flame regions shown in Figure 33. It is also seen from Figure 34 that the upper flame is thicker than the lower flame in agreement with the result obtained in the above section. Figure 35 shows the distribution of the mass fraction of the combustion product, which indicates the same thickening of the upper flame in the channel.

Conclusions

Ignition and combustion processes in a transonic accelerating mixing flow in a curved duct are studied by a
finite-volume method for the full elliptic Navier-Stokes equations. The method has been validated against boundary layer types of solutions. Computations for the flow in curved channels show surprisingly that the transverse pressure gradient does not directly affect the flame structure significantly. However, the velocity nonuniformity due to the transverse pressure gradient thickens the flame in the low speed region and appear to increase the combustion globally compared to the situation in a channel without transverse pressure gradient. Further detailed computation and analysis are needed to investigate the dependence of ignition and flame structures on the flow conditions and chemical kinetics of the fuel in order to explore the feasibility and technological advantages of the turbine-burner concept in the application of jet propulsion and ground power generation.

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