1 Summary

A non-ideal gas model has been developed and retro-fitted into the MSES viscous/inviscid multi-element airfoil program. The specific applications targeted are compressible airfoil flows in wind tunnels employing heavy gases. The particular gas modeled in this work has been sulfur hexafluoride (SF$_6$), although most heavy gases could be implemented if adequate state and caloric data were available.

Numerical predictions with MSES indicate that the non-ideality of SF$_6$ significantly influences airfoil behavior in transonic flows, especially at the higher total pressures envisioned for pressurized tunnels. The dominant effect is that for a given freestream Mach number, local Mach numbers in supersonic zones are lower, and shocks are correspondingly weakened. Another (but apparently smaller) effect is that for a given edge Mach number, a boundary layer in a heavy gas is theoretically somewhat more resistant to an adverse pressure gradient due to reduced adiabatic heating near the wall.

As pointed out by Wagner and Schmidt [1], transonic small-disturbance theory is valid for non-ideal gases. Similarity between two flows can be obtained if the transonic similarity parameter

$$K \equiv \frac{1 - M^2}{[M^2(\gamma' + 1)]^{2/3}}$$

is matched, and if the pressure coefficients are scaled by the factor

$$A \equiv (\gamma' + 1)\frac{M^2}{1 - M^2}$$

so that the quantity $AC_L$ must also be matched between the two flows. The parameters $K$ and $A$ above are defined in terms of an "equivalent" ratio of specific heats $\gamma'$, which is derived in Appendix B for the second-order small-disturbance formulation employed in MSES.

Although similarity between ideal and non-ideal inviscid transonic flows is rigorous in the context of transonic small-disturbance theory, a similarity rule cannot be formulated for viscous transonic flows. In addition to the Reynolds number $Re$, Appendix C shows that an additional parameter $\gamma_v$ is introduced. This depends on the gas properties and local Mach number, and scales the effect of the local Mach number on the displacement thickness. It therefore affects viscous displacement effects and boundary layer response to pressure gradients in compressible flows. It is highly unlikely that the parameters $M$, $\gamma'$, $Re$, and $\gamma_v$ can all be combined into one similarity rule for viscous transonic flows. Fortunately, numerical experiments indicate that matching $K$, $AC_L$, and $Re$ (or $M^*$, $CL$, and $Re$) still gives good correspondence between air and heavy-gas flows. Apparently, the effect of $\gamma_v$ is not nearly as significant as the other three parameters.

Figure 1 compares $C_p$ vs $x/c$ curves for the RAE 2822 airfoil [2] at $M = 0.735$ for air, for SF$_6$ at 1 atm, and for SF$_6$ at 3 atm. Figure 2 makes the comparison at a fixed $M^* = 0.765$ instead of a fixed $M$. Figure 3 in turn makes the comparison at a fixed $K$ and $AC_L$ (corresponding to $M = 0.735$ and $CL = 0.743$ for air). Clearly, matching $M^*$ or $K$ is more appropriate for evaluating
transonic flow characteristics. To illustrate further, drag-divergence behavior for air, $SF_6$ (1 atm), and $SF_6$ (3 atm) is shown versus $M$ and $M^*$ in Figures 4 and 5. As expected from the $C_p$ comparisons, the effects of the type of gas on transonic drag rise are much smaller if $M^*$ is used as the compressibility parameter in lieu of $M$. The Mach sweep results were not performed at fixed $K$ and $ACL$, since it is not clear how to scale the profile drag coefficient $C_D$ over this sweep. In principle, the pressure drag should be scaled by $A$, while the friction drag should perhaps be left unscaled. However, it is impossible to separate these drag components in an experiment, since only the total drag is obtained from a wake survey.

For high-lift configurations, small-disturbance theory is obviously invalid, but numerical studies indicate that matching $K$ and $ACL$ (or alternatively matching $M^*$ and $CL$) still gives a reasonably good match between air and heavy-gas flows. Figure 6 shows the inviscid $C_p$ distributions over a slatted two-element airfoil described in reference [3]. A freestream Mach number of $M = 0.30$ in air produces a fairly strong shock on the slat and a somewhat weaker shock on the main element. Figure 7 compares the $C_p$ distributions on the slat for the three gas cases at a fixed sonic Mach number $M^* = 0.3257$ (corresponding to $M = 0.30$ for air) and $CL = 2.85$. The comparison is quite reasonable. It should be stressed again that simply matching the usual freestream Mach number $M = V_\infty/\alpha_\infty$ and unscaled $CL$ gives a very poor match in all cases, except of course in effectively incompressible flows where any gas non-ideality is irrelevant.
Figure 2: $C_p$ distributions for RAE 2822 airfoil at $M^* = 0.765$ for air, $SF_6$ (1 atm), and $SF_6$ (3 atm). $C_L = 0.743$, $Re = 6.2$ million.

Figure 3: $C_p$ distributions for RAE 2822 airfoil at $K = 0.3867$ for air, $SF_6$ (1 atm), and $SF_6$ (3 atm). $AC_L = 2.095$, $Re = 6.2$ million.
Figure 4: RAE 2822 drag-divergence behavior versus $M$ for air, $SF_6$ (1 atm), and $SF_6$ (3 atm). $C_L = 0.743$, $Re = 6.2$ million.

Figure 5: RAE 2822 drag-divergence behavior versus $M^*$ for air, $SF_6$ (1 atm), and $SF_6$ (3 atm). $C_L = 0.743$, $Re = 6.2$ million.
Figure 6: $C_p$ distributions for slatted airfoil in air.

Figure 7: $C_p$ distributions over slat at $M^* = 0.3257$ and $C_L = 2.85$ for air, $SF_6$ (1 atm), and $SF_6$ (3 atm).
The bulk of the heavy-gas model development and application to transonic, inviscid flows is documented in the SM Thesis of Marc Schafer, which is attached as Appendix A. As mentioned previously, Appendix B derives the farfield behavior of a non-ideal airfoil flow. This was required for implementation of new outer boundary conditions for the MSES code. Appendix C derives the shape parameter compressibility correction for an adiabatic boundary layer in non-ideal flow. This was required to implement new heavy-gas correlations for the MSES integral boundary layer formulation.

References


Appendix A
Modeling of Heavy Gas Effects on Airfoil Flows

by

Marc Alan Schafer

Submitted to the Department of Aeronautics and Astronautics
on May 3, 1992
in partial fulfillment of the requirements for the degree of
Master of Science in Aeronautics and Astronautics

Thermodynamic models were constructed for a calorically imperfect gas and for
a non-ideal gas. These were incorporated into a quasi one dimensional flow solver to
develop an understanding of the differences in flow behavior between the new models and
the perfect gas model. The models were also incorporated into a two dimensional flow
solver to investigate their effects on transonic airfoil flows. Specifically, the calculations
simulated airfoil testing in a proposed high Reynolds number heavy-gas test facility. The
results indicated that the non-idealities caused significant differences in the flow field,
but that matching of an appropriate non-dimensional parameter led to flows similar to
those in air.

Thesis Supervisor: Mark Drela,
Associate Professor of Aeronautics and Astronautics
Acknowledgments

I would like to express my thanks to all those who made this thesis possible. First, to Mark Drela whose brilliance and ingenuity have served as an inspiration in all of my studies. Also, to Harold 'Guppy' Youngren whose leadership during the Daedalus project helped me to realize what it really means to be an engineer.

I would also like to thank my parents and the rest of my family. Without your support, I never would have made it as far as I have.

My appreciation also goes to the NASA Ames research center and the NDSEG fellowship program without whose financial support this thesis would never have happened.
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Chapter 1
Introduction

In the past few decades, the design and development of large transport aircraft has relied on wind tunnel data taken at significantly lower Reynolds numbers than those found in operation. The drawbacks of this subscale data become apparent when one considers phenomena such as attachment line transition or similar aspects of boundary layer behavior at high Reynolds numbers.

The need for accurate wind tunnel data clearly mandates the construction of a suitable high Reynolds number test facility. However, the cost of building a large atmospheric tunnel and large tunnel models is prohibitive. Higher Reynolds numbers are often achieved by pressurizing tunnels to effectively increase the density of the air. This alternative is practical only up to a point.

A potential solution following the same basic idea relies upon the use of gases with significantly higher molecular weights than air. Candidate gases include Freon-12 or Sulfur Hexafluoride ($SF_6$), but the use of non-breathable gases clearly causes some problems. These problems will likely be insignificant to the cost and operational advantages of such a facility. Combining heavy gases with pressurization would allow test Reynolds numbers comparable to those on large transports in flight [1].

One complication is that Freon and $SF_6$ have significantly different thermodynamic properties than air, especially at elevated pressures. Heavy gases do not follow the ideal equation of state $P = \rho RT$ nearly as well as air does, nor do they maintain a constant ratio of specific heats $\gamma \equiv c_p/c_v$ over any significant temperature range. The following discussion will attempt to quantify the potential importance of these effects through a computational study.
Chapter 2
Real Gases

The thermodynamic relations specifically subject to real gas effects are the state equation

\[ p = \rho RT \] (2.1)

and the caloric equation,

\[ h \equiv \int c_p dT = c_p T \] (2.2)

these particular forms only being valid for a perfect gas. Real gas effects may be divided into two categories:

1. Calorically imperfect gases for which \( c_p \) depends on temperature, but which still satisfy equation (2.1).

2. Non-ideal gases for which \( c_p \) depends on both pressure and temperature, and equation (2.1) no longer holds.

The first effect results from the introduction of multiple vibrational modes for polyatomic molecules which become more important at higher temperatures. The second effect depends on intermolecular forces which become stronger as a gas moves towards liquefaction, ie. higher pressures and lower temperatures.

2.1 Calorically Imperfect Gases

The only difference between a perfect and an imperfect gas stems from the dependence of \( c_p \) on temperature in the imperfect case. A cursory examination of experimental data for \( SF_6 \) shows that, in the range of temperatures likely to be found in a wind tunnel
test, this dependence is linear in temperature.

\[ c_p(T) = a + bT \]  

(2.3)

Therefore, equation (2.2) becomes

\[ h(T) = aT + \frac{bT^2}{2} \]  

(2.4)

which may be easily inverted to find \( T(h) \).

\[ T(h) = -\frac{a}{b} + \sqrt{\left(\frac{a}{b}\right)^2 + \frac{2h}{b}} \]  

(2.5)

2.2 Non-Ideal Gases

The state equation for a perfect gas (2.1) derives from a kinetic model of gas molecules which assumes that the molecules are point masses and that they do not exert any forces on one another except instantaneously during collisions. Clearly these assumptions become less accurate as the molecular weight of the gas increases. Van der Waals's equation

\[ \left( p + \rho^2\alpha \right)(1 - \rho\beta) = \rho RT \]  

(2.6)

contains two correction to equation (2.1): \( \alpha \) corrects the pressure to account for inter-molecular attraction, and \( \beta \) corrects for the volume of the molecules themselves.

Using a non-ideal state equation like Van der Waals's causes many serious complications as enthalpy, \( c_p \), \( \gamma \), etc. now depend on pressure as well as temperature. Despite these complications, enthalpy and entropy must remain state variables regardless of the form of the state equation. That is, local entropy and enthalpy must depend only on the local pressure and temperature and not on the upstream conditions (ie. the gas history).

Liepmann and Roshko [2] equate this condition with the requirement that a canonical equation of state must have one of these four forms:

\[ e = e(s, \rho) \]  

(2.7)
\[ h = h(s, p) \quad (2.8) \]
\[ f = f(T, \rho) \quad (2.9) \]
\[ g = g(T, p) \quad (2.10) \]

Here \( e = h - p/\rho \) is the usual internal energy, \( f \equiv e - Ts \) is the free energy, and \( g \equiv h - Ts \) is the free enthalpy.

For a conventional flow solver, the enthalpy definition (2.8) appears best; however, specifying the state in this specific form is not convenient because the entropy \( s \) is not readily available to the flow solver. Liepmann and Roshko propose a more suitable form

\[ \frac{p}{\rho RT} = Z(p, T) \quad (2.11) \]

which requires \( T(\rho, h) \) to have a form which makes \( h \) a state variable.

For a Van der Waals's gas

\[ Z = \frac{1}{1 - \beta \rho - \frac{\alpha \rho}{RT}} \quad (2.12) \]

which clearly approaches the ideal state equation for \( \alpha, \beta \to 0 \). For typically small values of \( \alpha \) and \( \beta \)

\[ Z \simeq 1 + \rho \left( \beta - \frac{\alpha}{RT} \right) \simeq 1 + \frac{p}{RT} \left( \beta - \frac{\alpha}{RT} \right) \quad (2.13) \]

where the second approximation is made to make \( Z = Z(p, T) \) explicitly. Liepmann and Roshko write equation (2.13) in more general form as

\[ Z = 1 + \frac{p}{p_c} \phi \left( \frac{T_c}{T} \right) \quad (2.14) \]

with \( p_c \) and \( T_c \) being the critical pressure and temperature of the gas, and \( \phi \) evidently being a universal function which they tabulate for gases other than air but with approximately the same molecular weight. For heavier gases such as \( SF_6 \) it is best to fit a curve to experimental data as explained in Appendix A. For \( SF_6 \), a good curve fit takes the form

\[ \phi \left( \frac{T_c}{T} \right) = c_2 \left( \frac{T_c}{T} \right)^2 + c_1 \left( \frac{T_c}{T} \right) + c_0 \quad (2.15) \]

It is now necessary to determine the specific heat capacity \( c_p(p, T) \) so that the enthalpy function \( h(p, T) \) can be obtained. Liepmann and Roshko combine two forms of the
equation of state \( h(p, T) \) and \( s(p, T) \) into the fundamental reciprocity relation between \( h(p, T) \) and \( \rho(p, T) \)

\[
\frac{\partial h}{\partial p} = \frac{1}{\rho} - T \frac{\partial (1/\rho)}{\partial T}
\]  

(2.16)

which is valid for any gas. Combining this with the state equation (2.11) gives

\[
\frac{\partial h}{\partial p} = -\frac{RT^2}{p} \left( \frac{\partial Z}{\partial T} \right)_p = \frac{RT_c}{p_c} \phi' \left( \frac{T_c}{T} \right) \equiv F(T) \]

(2.17)

Since \( \partial h/\partial p = F(T) \) only depends on the temperature, both \( h \) and \( c_p \) must be linear in the pressure as follows.

\[
h(p, T) = \int c_p(T) \, dT + p F(T)
\]

(2.18)

\[
c_p(p, T) = \frac{\partial h}{\partial T}
\]

(2.19)

\[
c_p(T) + p \frac{dF}{dT}
\]

(2.20)

\[
c_p(T) = c_p(T) - R \frac{p}{p_c} \frac{T_c^2}{T^2} \phi'' \left( \frac{T_c}{T} \right)
\]

(2.21)

As in the case of the calorically imperfect gas, \( c_p(T) \) has the form

\[
c_p(T) = a + bT
\]

(2.22)

Substituting this into the enthalpy equation gives

\[
h(p, T) = aT + \frac{bT^2}{2} + \frac{pRT_c}{p_c} \phi' \left( \frac{T_c}{T} \right)
\]

(2.23)

It is also possible to determine the caloric equation by expressing the internal energy \( e \) as \( e(\rho, T) \) [3].
Chapter 3
Solving the Euler Equations

These gas models may be readily integrated into an existing flow solver which solves the integral form of the steady Euler equations:

\[ \int \rho \mathbf{u} \cdot \hat{n} \, dA = 0 \]  
(3.1)

\[ \int (\rho \mathbf{u} \cdot \hat{n} \mathbf{u} + p \hat{n}) \, dA = 0 \]  
(3.2)

\[ h_0 = h + \frac{|\mathbf{u}|^2}{2} = \text{constant} \]  
(3.3)

These equations are exact for any fluid flow, but must be supplied with a state equation to relate the pressure \( p \) to the enthalpy \( h \) and the density \( \rho \). In addition, the upwinding scheme used to capture the shocks requires the local Mach number while the boundary conditions and evaluation of shock losses require the local stagnation conditions.

It is desirable to nondimensionalize the equations, and the following scheme is used where \( () \) denotes the dimensional quantity and \( ()_{\text{ref}} \) denotes a reference quantity:

\[ p = \frac{\hat{p}}{\rho_{\text{ref}}} \]
\[ \rho = \frac{\hat{\rho}}{\rho_{\text{ref}}} \]
\[ T = \frac{\hat{T}}{T_{\text{ref}}} \]
\[ h = \frac{\hat{h}}{\rho_{\text{ref}}/\rho_{\text{ref}}} \]

Furthermore, \( c_p \), \( c_v \), and \( R \) are nondimensionalized using \( R \) resulting in several new nondimensional parameters:

\[ \alpha = \frac{a}{R} \]
\[ \beta = \frac{bT_{\text{ref}}}{2a} \]
\[ \tau = \frac{P_{\text{ref}}}{P_c} \]
\[ \tau = \frac{T_{\text{ref}}}{T_c} \]
For the results presented here, the reference conditions are chosen to be stagnation conditions.

### 3.1 Calorically Imperfect Gas

The nondimensional form of the caloric equation which governs the behavior of the imperfect gas is:

\[
h(r) = \int c_p \, dT = aT + a\beta T^2
\]

(3.4)

(3.5)

which may be inverted to give \( T \) as a function of \( h \).

\[
T(h) = \frac{-1 + \sqrt{1 + 4\beta h/a}}{2\beta}
\]

(3.6)

With \( T \) obtained from \( h \), \( p \) may be determined using the ideal gas law (2.1) and a specified value of \( \rho \). The local Mach number comes from the familiar definition of the speed of sound:

\[
a^2 \equiv \left[ \frac{\partial p}{\partial \rho} \right] = \gamma T
\]

(3.7)

The local value of \( \gamma \) may be found from equation (2.3).

\[
\gamma = \frac{c_p}{c_v} = \frac{\alpha + 2\alpha\beta T}{1 - \alpha - 2\alpha\beta T}
\]

(3.8)

The last remaining difficulty is the determination of the isentropic relations between pressure, density, and temperature. These relations are necessary to calculate stagnation conditions from flow conditions. The familiar perfect gas relations

\[
\frac{T}{T_0} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{-1} \quad \frac{\rho}{\rho_0} = \left(\frac{T}{T_0}\right)^{\frac{\gamma-1}{\gamma}} \quad \frac{p}{p_0} = \left(\frac{T}{T_0}\right)^{\frac{\gamma}{\gamma-1}}
\]

do not hold for a calorically imperfect gas.

The proper forms are obtained from the formal statement,

\[
dh = T \, ds + \frac{dp}{\rho}
\]

(3.9)
and for an isentropic process $ds = 0$:

$$dh = \frac{dp}{\rho}$$

(3.10)

From the definition of enthalpy $dh = c_p dT$, and for an ideal gas $p/\rho = T$, so equation (3.10) becomes

$$\frac{c_p(T) dT}{T} = \frac{dp}{p}$$

(3.11)

Integrating this equation gives

$$\frac{p_0}{p} = \exp(-\alpha \log T + 2\alpha \beta (1 - T))$$

(3.12)

and the isentropic density relation then follows directly from the state equation.

$$\frac{\rho}{\rho_0} = \frac{p}{p_0} \frac{T(h_0)}{T(h)}$$

(3.13)

Strictly speaking, solution of the Euler equations requires nothing else. However, if a Newton-Raphson technique is used, all of the necessary equations must be linearized for the Jacobian matrix. In the case of the calorically imperfect gas, the equations are slightly more complicated than for a perfect gas, but they may still all be written explicitly. Therefore the linearizations are easily done by differentiating the relevant equations.

### 3.2 Non-Ideal Gas

The nondimensional equations describing the non-ideal gas are the state equation

$$\frac{p}{\rho T} = \frac{1 + \rho \pi \phi(\frac{\rho}{T})}{Z_0}$$

(3.14)

and the caloric equation.

$$h(p, T) = \left[ \alpha T + \alpha \beta T^2 + p \pi \phi'(\frac{1}{\pi T}) \right] \frac{1}{Z_0}$$

(3.15)

$Z_0$ is another parameter which may be described in terms of $\pi$ and $\tau$.

$$Z_0 = \frac{p_0}{\rho_0 T_0} = 1 + p_0 \pi \phi(\frac{1}{\pi T_0})$$

(3.16)
The non-ideal gas presents some difficulty as the enthalpy depends on the temperature and the pressure. Therefore, from equations (3.14) and (3.15), \( p \) and \( T \) may be found using a Newton-Raphson system to drive the following residuals to zero.

\[
R_1(p, T) = \frac{p}{\rho T} - \frac{1 + p\pi \phi\left(\frac{1}{T}\right)}{Z_0} \tag{3.17}
\]

\[
R_2(p, T) = h - \left[ \alpha T + \beta T^2 + \rho \pi \phi'\left(\frac{1}{T}\right) \right] \frac{1}{Z_0} \tag{3.18}
\]

The local Mach number depends on the speed of sound which must be found from the definition:

\[
a^2 = \frac{\partial p}{\partial \rho} \tag{3.19}
\]

This is calculated as follows:

\[
dp = \frac{\partial p}{\partial \rho} \frac{d\rho}{dh} + \frac{\partial p}{\partial h} \frac{dh}{dh} \tag{3.20}
\]

but \( dh = dp/\rho \) for an isentropic process, and hence

\[
a^2 = \frac{\partial p}{\partial \rho} \frac{1}{1 - \frac{\partial h}{\partial \rho}} \tag{3.21}
\]

The local \( \gamma \) really has no meaning and need not be calculated.

The extra complexity of the non-ideal gas appears in the calculation of the sensitivities. Since \( p \) and \( T \) are found by an iterative process they must be found by perturbing the Jacobian matrix of the converged Newton-Raphson system. A perturbation in \( h \) and \( \rho \) is related to a perturbation in \( p \) and \( T \) by the condition that the \( R(p, T, h, \rho) \) must remain zero.

\[
\begin{bmatrix}
\delta R_1 \\
\delta R_2
\end{bmatrix} = 0 = \begin{bmatrix}
\frac{\partial R_1}{\partial h} & \frac{\partial R_1}{\partial \rho} \\
\frac{\partial R_2}{\partial h} & \frac{\partial R_2}{\partial \rho}
\end{bmatrix} \begin{bmatrix}
\delta h \\
\delta \rho
\end{bmatrix} + \begin{bmatrix}
\frac{\partial R_1}{\partial p} & \frac{\partial R_1}{\partial T} \\
\frac{\partial R_2}{\partial p} & \frac{\partial R_2}{\partial T}
\end{bmatrix} \begin{bmatrix}
\delta p \\
\delta T
\end{bmatrix} \tag{3.22}
\]

Numerically inverting this system gives the required derivatives.

\[
\begin{bmatrix}
\delta p \\
\delta T
\end{bmatrix} = \begin{bmatrix}
\frac{\partial p}{\partial h} & \frac{\partial p}{\partial \rho} \\
\frac{\partial T}{\partial h} & \frac{\partial T}{\partial \rho}
\end{bmatrix} \begin{bmatrix}
\delta h \\
\delta \rho
\end{bmatrix} \tag{3.23}
\]

The second derivatives are found in a similar fashion starting instead with \( \frac{\partial R_1}{\partial h} \) and \( \frac{\partial R_1}{\partial \rho} \) as the residuals. Using a subscript notation for the derivatives (\( \frac{\partial}{\partial h} \equiv p_h \)):

\[
\begin{bmatrix}
\delta R_{1h} \\
\delta R_{2h}
\end{bmatrix} = 0 = \begin{bmatrix}
\frac{\partial R_{1h}}{\partial h} & \frac{\partial R_{1h}}{\partial \rho} \\
\frac{\partial R_{2h}}{\partial h} & \frac{\partial R_{2h}}{\partial \rho}
\end{bmatrix} \begin{bmatrix}
\delta h \\
\delta \rho
\end{bmatrix} + \begin{bmatrix}
\frac{\partial R_{1h}}{\partial p_h} & \frac{\partial R_{1h}}{\partial T_h} \\
\frac{\partial R_{2h}}{\partial p_h} & \frac{\partial R_{2h}}{\partial T_h}
\end{bmatrix} \begin{bmatrix}
\delta p_h \\
\delta T_h
\end{bmatrix} \tag{3.24}
\]
A similar system with $R_{1p}$ and $R_{2p}$ as residuals is also formed. As above, numerically inverting gives $\frac{\partial h}{\partial T} = \frac{\partial p}{\partial T}$, $\frac{\partial p}{\partial T} = \frac{\partial h}{\partial T}$, etc. These manipulations are implemented in the source code in Appendix B.

The last remaining task is calculation of the stagnation conditions and, again, it is not possible to find an analytic expression. Another Newton-Raphson system is constructed where the first residual comes from equation (3.15):

$$R_1 = h_0 - h(p,T)$$  \hspace{1cm} (3.25)

The second residual is derived by rearranging equation (3.9)

$$ds = \frac{dh}{T} + \frac{dp}{pT}$$  \hspace{1cm} (3.26)

$$= \frac{c_p}{T}dT + \frac{d(pF)}{T} - \frac{dp}{p}$$  \hspace{1cm} (3.27)

$$= \frac{c_p}{T}dT + \frac{d(p\frac{1}{\tau T} \phi')}{p} - \pi d(p\phi) - \frac{dp}{p}$$  \hspace{1cm} (3.28)

Integrating gives:

$$s(p,T) = \int \frac{c_p}{T}dT + p\pi \left[ \frac{1}{\tau T} \phi' - \phi \right] - ln(p)$$  \hspace{1cm} (3.29)

The second residual may then be formed

$$R_2 = s_1 - s(p,T)$$  \hspace{1cm} (3.30)

where $s_1$ is the entropy of the static conditions.

Driving these two residuals to zero gives the stagnation conditions $p_0, T_0$. The derivatives $\frac{\partial h}{\partial p}, \frac{\partial p}{\partial h}$, etc, needed for the Newton-Raphson solver may then be found by perturbing the converged Jacobian matrix and relating the resulting derivatives to the static conditions through the chain rule and equations (3.15) and (3.29). This process is identical to the one used above to find $p$ and $T$ and their derivatives.
Chapter 4

Results

After developing the models for the calorically imperfect and non-ideal gases, the next step was to evaluate the differences these changes caused in inviscid flows. The primary quantities of interest are the location of shocks and their strength which is defined as the ratio of stagnation pressures across the shock. For a perfect gas, the shock strength may be expressed as a function of the upstream Mach number $M_1$:

$$
\frac{P_{02}}{P_{01}} = \left[1 + \frac{2\gamma}{\gamma + 1} (M_1^2 - 1)\right]^{1/(\gamma - 1)} \left[\frac{(\gamma + 1)M_1^2}{(\gamma - 1)M_1^2 + 2}\right]^{\gamma/(\gamma - 1)}
$$

(4.1)

However, for the non-ideal gas, this relation must be calculated numerically.

Figure 4.1: Stagnation Pressure Ratio (Strength) vs. Upstream Mach No. for Air and $SF_6$ at 1atm and 3atm
4.1 One Dimensional Duct Flow

The first comparison of the different gas models was a study of the flow in a converging/diverging nozzle using a quasi one dimensional Euler solver. This flow is characterized by sonic flow at the throat with a shock downstream to match the specified exit pressure as shown in figure (4.2).

As a basis for comparison of the different gas models in a duct flow, the non-dimensional reference enthalpy \( h_0 p_0/p_0 \) was made equal for all three cases.

\[
\begin{align*}
h_0 &= \frac{\gamma}{\gamma - 1} \\
    &= \alpha(1 + \beta) \\
    &= \frac{\alpha(1 + \beta) + \pi \phi'(\frac{1}{\pi})}{Z_0}
\end{align*}
\]

With \( h_0 \) held constant, \( \gamma \) therefore depends on \( \alpha, \beta, \pi, \) and \( \tau \). The exit pressure ratio is also held constant. Under these conditions, the slope of the \( c_p \) versus \( T \) curve \( (\beta) \) had little or no effect on shock strength or position relative to the perfect gas as shown in figure (4.3).
For the non-ideal gas, \( \pi \) and \( \tau \) are not really independent parameters and may be combined into \( Z_0 \). Figure 4.4 shows the variation in shock strength and position as functions of \( Z_0 \) and the corresponding perfect gas results with \( \gamma \) adjusted to preserve the stagnation enthalpy as above. These plots clearly show that it is not possible to mimic the effects of the non-ideality by changing \( \gamma \) as in the case of the calorically imperfect gas. The difference in shock strength and position becomes larger and larger as the gas becomes less ideal.
The last test conducted with the one dimensional flow model was to determine the effects of the various gas models on the upwinding scheme needed for stability of the numerical scheme. The flow solver drives the momentum equation residual to zero,

\[ R_i \equiv \rho_i q_i A_i (\bar{q}_i - q_{i-1}) + \rho_i A_i - \rho_{i-1} A_{i-1} + \frac{\rho_i + \rho_{i-1}}{2} (A_i - A_{i-1}) \tag{4.5} \]

where the upwinded speed is defined as

\[ \bar{q}_i = q_i - \mu_i (q_i - q_{i-1}) \tag{4.6} \]

and \( \mu_i \) is non-zero only if \( M_i \) is greater than \( M_c \).

\[ \mu_i(M_i(q_i)) = \frac{K_\mu}{\gamma} \left[ 1 - \frac{M_i^2}{M_c^2} \right] \tag{4.7} \]

Initially, the exact \( \gamma \) was calculated at each node along with all the necessary linearizations and used in the upwinding scheme. Under these conditions, the flow solver converged with \( M_c \leq 1 \). However, the upwinding is relatively insensitive to the exact value of \( \gamma \) even though the stability analysis used to derive equation(4.7) ignored \( \gamma \) perturbations. Using a constant value of \( \gamma \) had absolutely no effect on the viable range for \( M_c \) or the rate of convergence.

4.2 Two Dimensional Results

The subroutine which appears in Appendix B was incorporated into MSES, the multi-element version of the two dimensional transonic airfoil design/analysis code ISES [4]. Numerical experiments carried out were limited to single-element inviscid cases to more clearly demonstrate the effect of the new gas model. Figure(4.5) shows an overlay of the Mach distributions for a test airfoil run in \( SF_6 \) at two different stagnation conditions and in air. All three cases are at matched freestream Mach number and lift coefficient. Note that they are not at the same angle of attack. The \( SF_6 \) is characterized by stagnation pressures of 1atm and 3atm and a stagnation temperature of 310K.

Airfoils tests in heavy gases will be much more worthwhile if some relationship may be found so that the tests reflect the airfoil performance in air. The only parameters
Figure 4.5: Comparison of Air and $SF_6$ at Fixed $M$ and $C_L$

which may be adjusted in a wind tunnel test are the Mach number, stagnation conditions, and angle of attack or $C_L$. Figure(4.5) shows an attempted match keeping $M$ and $C_L$ constant: clearly, this is not an effective technique. After a good deal of experimentatation, the best match was achieved by running the different gases at the same $M^*$ which is defined as the ratio of freestream velocity to the speed of sound at sonic conditions. Figure(4.6) shows the case in air from figure(4.5) compared with $SF_6$ (1atm and 3atm) at the same $M^*$.

Figure 4.6: Comparison of $SF_6$ at 1atm and 3atm to Air, $M^* = .740$, $C_L = .9$
A case with a weaker shock, figure 4.7 was used to further verify this relationship. The match is slightly worse, but this is to be expected because a weak shock is much more sensitive to small changes in $M$ than a strong one. As an alternative to matching $M^*$, Anderson [5] proposes matching the small disturbance similarity parameter $\kappa$ and $AC_L$ where

$$\kappa = \frac{1 - M_{\infty}^2}{(M_{\infty}^2(\gamma' + 1))^{3/2}}$$

$$A = \frac{M_{\infty}^2(\gamma' + 1)}{1 - M_{\infty}^2}$$

Figure 4.8: Comparison of $SF_0$ at 1atm and 3atm to Air, $\kappa = .439$, $AC_L = 2.18$
Chapter 5
Conclusions

The models derived above adequately describe the thermodynamic behavior of non-ideal and calorically imperfect gases. Despite some minor complications in linearizing these models, they were implemented in routines suitable for incorporation into existing flow solvers based on Newton's method. First, a quasi one-dimensional flow solver was used to examine the influence of the various non-dimensional parameters which govern the behavior of the different gases.

Transonic airfoil test cases for air and SF₆ were then used to study the influence of parameters which may be controlled in a wind tunnel experiment: stagnation pressure, freestream Mach number, and angle of attack. The goal of this study was to determine the conditions under which a wind tunnel test in a heavy gas would produce results comparable to those found in air. Matching $M^*$ and $C_L$ or $\kappa$ and $AC_L$ were both effective for the test cases presented here. Further study is necessary to determine which is best for multi-element cases.

The results are encouraging in that they definitely hint at the possibility of directly relating heavy gas test data to performance in air. It is first necessary to verify experimentally the model for SF₆, and to investigate the effects of non-ideal gases on viscous flows.
Appendix A

Curve Fit For $SF_6$ State Equation

A curve fit may be found for the function $\phi \left( \frac{T}{p} \right)$ for any gas given experimental state data. With the density ($\rho$) measured at a number of different pressures ($p$) and temperatures ($T$), a vector is defined containing the difference between the real gas and a perfect gas at each data point.

\[
\vec{Z} = \begin{bmatrix}
-\frac{p_1}{\rho_1 RT_1} - 1 \\
\vdots \\
-\frac{p_m}{\rho_m RT_m} - 1
\end{bmatrix}
\]  

(A.1)

Defining $\theta \equiv \frac{T}{p}$, the matrix $A$ contains the state information.

\[
A = \frac{1}{p_{ref}} \begin{bmatrix}
p_1 \theta_1^p & p_1 \theta_1^{p-1} & \cdots & p_1 \theta_1 & p_1 \\
\vdots & \vdots & \cdots & \vdots & \vdots \\
p_m \theta_m^p & p_m \theta_m^{p-1} & \cdots & p_m \theta_m & p_m
\end{bmatrix}
\]  

(A.2)

The goal is to find a state equation agreeing closely with the experimental data in $\vec{Z}$ but of the simple form:

\[
Z(p, T) = 1 + \frac{p}{p_{ref}} \begin{bmatrix}
C_n & C_{n-1} & \cdots & C_0
\end{bmatrix} \begin{bmatrix}
\theta^n \\
\theta^{n-1} \\
\vdots \\
1
\end{bmatrix}
\]  

(A.3)

Therefore

\[
\vec{Z} \approx \dot{A} \dot{C}
\]  

(A.4)

and $\dot{C}$ is found by the technique of linear regression:

\[
\dot{C} = (A^T A)^{-1} A^T \vec{Z}
\]  

(A.5)

The results presented in this thesis were based on a quadratic fit for $\phi$ from approximate data for $SF_6$. The required data may be found in [6].
Appendix B

MSES Subroutine for Non-Ideal Gas Model

subroutine hgparm(alfl,btal, taul, cc0,cc1,cc2, h0)

---

Initializes non-ideal gas routines.
Formulation derived in Schafer SM thesis.

Input:
- alfl: Constants for Cp(T) in caloric equation: Cp = a(1 + bT)
- betl
- taul: Constant in phi(T) in non-ideality factor Z(p,T)
- cc0: Constants defining phi(T) in polynomial form:
  - cc1
  - cc2: phi = c0 + c1(taul/T) + c2(taul/T)**2

Output:
- h0: Enthalpy at reference conditions p0, T0
- z0: Non-ideality factor Z(p0,T0) at reference conditions

Implicit real*4 (a-h,m,o-z)
Common /nongas/
& alf, bta, pi, tau, z0
Common /nonfit/
& c2, c1, c0

Put input parameters into common blocks
- alf = alfl
- bta = btal
- tau = taul
- c0 = cc0
- c1 = cc1
- c2 = cc2
- pi = 1.0

Calculate reference non-ideality factor and enthalpy
- z0 = 1.0 + pi*(c2/taul**2 + c1/tau + c0)
- h0 = (alfl*(1. + bta) + pi/tau*phi(1./tau)) / z0
subroutine nideal(hO,r,q, p ,p_r ,p_q, 
msq,msq_r,msq_q)

Calculates pressure and Mach number for specified
stagnation enthalpy, density, and speed.

Input:
hO stagnation enthalpy
r density
q speed

Output:
p pressure
p_r dp/dr
p_q dp/dq
msq square of Mach number M^2
msq_r dM^2/dr
msq_q dM^2/dq

implicit real*4 (a-h,m-o-z)

set static enthalpy
h = hO - 0.5*q**2
h_q = -q

set pressure and temperature and derivatives
call ngsaspt(h,r,p,p_r,p_h,p_rr,p_hh,p_rh, 
& t,t_r,t_h,t_rr,t_hh,t_rr)
p_q = p_h*h_q

set speed of sound squared: a^2 = dp/dr (at constant s)
asq = p_r / (1. - p_h/r)
asq_r = p_rr / (1. - p_h/r)
& - p_r / (1. - p_h/r)**2 *(p_h/r**2 - p_rh/r)
asq_h = p_rh / (1. - p_h/r)
& + p_r / (1. - p_h/r)**2 *p_hh/r
asq_q = asq_h*h_q

set Mach number squared
msq = q**2/asq
msq_r = -msq/asq * asq_r
msq_q = -msq/asq * asq_q + 2.*q/asq

return
end

subroutine ngsaspt(h,r,p,p_r,p_h,p_rr,p_hh,p_rh,
Calculates pressure and temperature for specified static enthalpy and density.

Input:
- \( h \) enthalpy
- \( r \) density

Output:
- \( p \) pressure
- \( p_r \) \( \frac{dp}{dr} \)
- \( p_h \) \( \frac{dp}{dh} \)
- \( p_{rr} \) \( \frac{d^2p}{dr^2} \)
- \( p_{hh} \) \( \frac{d^2p}{dh^2} \)
- \( p_{rh} \) \( \frac{d^2p}{dr dh} \)
- \( t \) temperature
- \( t_r \) \( \frac{dt}{dr} \) etc.

Implicit real*4 (a-h,m,o-z)
Dimension a(2,2), ai(2,2), aih(2,2), air(2,2),
& b(2,2), bh(2,2), br(2,2)
Common /nongas/
& alf, bta, pi, tau, z0

C---- Newton convergence tolerance
data eps /5.0E-6/

C---- Initial guess from imperfect ideal gas
if(bta.eq.0.0) then
  t = h/alf
else
  t = (-1.0 + sqrt(1.0 + 4.0*bta*alf)) / (2.0*bta)
endif
p = ret

C---- Newton loop to converge on correct p,t
itcon = 15
do 100 iter=1, itcon

C---- Set and linearize non-ideality factor Z(p,t)
ttc = 1./(tau)
ttc_t = -1./(tau**2)

Z = 1. + p*pi*phi(ttc)
Z_p = pi*phi(ttc)
Z_t = pi*phi(ttc)*ttc_t

C---- Residual 1: State equation
res1 = p/(ret) - z /z0
r1_p = 1./(ret) - z_p/z0
r1_t = -p/(ret*2) - z_t/z0

C
\[
\begin{align*}
tm1 &= \frac{(\alpha t + \alpha bta t^2)}{z_0} \\
tm1_p &= 0. \\
tm1_t &= \frac{(\alpha + 2.\alpha bta t)}{z_0} \\
tm2 &= \frac{p^2 \pi / \tau \phi(tc)}{z_0} \\
tm2_p &= \frac{p^2 \pi / \tau \phi(tc)}{z_0} \\
tm2_t &= \frac{p^2 \pi / \tau \phi(tc)}{z_0} \\
\end{align*}
\]

c--- residual 2: caloric equation
\[
\begin{align*}
res2 &= h - (tm1 + tm2) \\
r2_p &= -(tm1_p + tm2_p) \\
r2_t &= -(tm1_t + tm2_t) \\
\end{align*}
\]

c--- set Jacobian matrix
\[
\begin{align*}
a(1,1) &= r1_t \\
a(1,2) &= r1_p \\
a(2,1) &= r2_t \\
a(2,2) &= r2_p \\
\end{align*}
\]

c--- find inverse Jacobian matrix
\[
\begin{align*}
detinv &= 1.0 / (a(1,1)*a(2,2) - a(1,2)*a(2,1)) \\
a(1,1) &= a(2,2)*detinv \\
a(2,2) &= a(1,1)*detinv \\
a(1,2) &= -a(1,2)*detinv \\
a(2,1) &= -a(2,1)*detinv \\
\end{align*}
\]

c--- set Newton changes
\[
\begin{align*}
dt &= -(a(1,1)*res1 + a(1,2)*res2) \\
dp &= -(a(2,1)*res1 + a(2,2)*res2) \\
\end{align*}
\]

c--- update variables
\[
\begin{align*}
t &= t + rlx*dt \\
p &= p + rlx*dp \\
\end{align*}
\]

c--- convergence check
\[
\begin{align*}
\text{if } & (\text{abs(dp/p)} \leq \text{eps}) \text{ and } (\text{abs(dt/t)} \leq \text{eps}) \text{ goto 3} \\
100 \ & \text{continue} \\
\end{align*}
\]

write(*,*) 'NGASPT: Convergence failed.'
write(*,*) 'dp dt :', dp, dt
write(*,*) 'p T h r:', p, t, h, r

3 \ & \text{continue} \\

c--- set residual derivatives wrt input r,h variables
\[
\begin{align*}
ri_r &= -p/(r^2) \\
ri_h &= 0. \\
\end{align*}
\]
\[ r_{2_r} = 0. \]
\[ r_{2_h} = 1. \]

\[
\begin{align*}
b(1,1) &= r_{1_r} \\
b(1,2) &= r_{1_h} \\
b(2,1) &= r_{2_r} \\
b(2,2) &= r_{2_h}
\end{align*}
\]

\[ \text{c} \]
\[ \text{c} \quad \text{set } p,t \text{ derivatives wrt } r,h \]
\[
\begin{align*}
t_r &= - (a(1,1) \cdot b(1,1) + a(1,2) \cdot b(2,1)) \\
t_h &= - (a(1,1) \cdot b(1,2) + a(1,2) \cdot b(2,2)) \\
p_r &= - (a(2,1) \cdot b(1,1) + a(2,2) \cdot b(2,1)) \\
p_h &= - (a(2,1) \cdot b(1,2) + a(2,2) \cdot b(2,2))
\end{align*}
\]

\[ \text{c} \]
\[ \text{c} \quad \text{set second residual derivatives wrt } r,h \]
\[
\begin{align*}
ttc &= 1. / (\tau * t) \\
ttc_t &= -1. / (\tau * t * t^2) \\
ttc_tt &= 2. / (\tau * t * t^3)
\end{align*}
\]

\[
\begin{align*}
z &= 1. + p * \pi * \phi(ttc) \\
z_p &= \pi * \phi(ttc) \\
z_{pt} &= \pi * \phi'(ttc) * ttc_t \\
z_{pp} &= 0. \\
z_t &= \pi * \phi'(ttc) * ttc_t \\
z_{tt} &= \pi * \phi''(ttc) * ttc_t * ttc_t + \phi'(ttc) * ttc_{tt}
\end{align*}
\]

\[ \text{c} \]
\[
\begin{align*}
r_1 &= p / (r * t) - z / z_0 \\
r_{1_p} &= 1. / (r * t) - z_p / z_0 \\
r_{1_{pt}} &= -1. / (r * t * t^2) - z_{pt} / z_0 \\
r_{1_{pp}} &= - z_{pp} / z_0 \\
r_{1_t} &= -p / (r * t * t^2) - z_t / z_0 \\
r_{1_{tt}} &= 2. * p / (r * t * t^3) - z_{tt} / z_0 \\
r_{1_r} &= -p / (r * t * t^2) \\
r_{1_h} &= 0. \\
r_{1_{hp}} &= 0. \\
r_{1_{ht}} &= 0. \\
r_{1_{rp}} &= -1. / (r * t * t^2) \\
r_{1_{rt}} &= p / (r * t * t * t^2) \\
r_{1_{rr}} &= 2. * p / (r * t * t^3)
\end{align*}
\]

\[ \text{c} \]
\[
\begin{align*}
tm1 &= (a + a * \alpha * \beta * t * t) / z_0 \\
tm1_t &= (a + 2. * a * \alpha * \beta * t) / z_0 \\
tm1_tt &= (2. * a * \alpha * \beta) / z_0 \\
tm1_{pt} &= 0. \\
tm1_p &= 0. \\
tm1_{pp} &= 0.
\end{align*}
\]

\[ \text{c} \]
\[
\begin{align*}
tm2 &= p * \pi / \tau * \phi(ttc) / z_0 \\
tm2_p &= \pi / \tau * \phi(ttc) / z_0 \\
tm2_{pt} &= \pi / \tau * \phi'(ttc) * ttc_t / z_0 \\
tm2_{pp} &= 0. \\
tm2_t &= p * \pi / \tau * \phi'(ttc) * ttc_t / z_0 \\
tm2_{tt} &= p * \pi / \tau * \phi''(ttc) * ttc_t * ttc_t +
\end{align*}
\]
& phidd(ttc)*ttc_tt) / Zo

c
r2 = h - (tm1 + tm2)
r2_p = (tm1_p + tm2_p)
r2_t = (tm1_t + tm2_t)
r2_h = 1.
c
c---- set and linearize new residuals: r1h = dr1/dh = 0, r2h = dr2/dh = 0

ph = p_h
th = t_h
c
r1h = r1_p*ph + r1_t*th + r1_h
r1h_ph = r1_p
r1h_th = r1_t
r1h_p = r1_pp*ph + r1_pt*th + r1_hp
r1h_t = r1_pt*ph + r1_tt*th + r1_ht
r1h_h = 0.
r1h_r = -ph/(r**2*t) + th*p/(r**2*t**2)
c
c
r2h = 1. - tm1_t*th - tm1_p*ph - tm2_t*th - tm2_p*ph
r2h_ph = -tm1_p - tm2_p
r2h_th = -tm1_t - tm2_t
r2h_p = -tm1_pt*th - tm1_pp*ph - tm2_pt*th - tm2_pp*ph
r2h_t = -tm1_tt*th - tm1_pt*ph - tm2_tt*th - tm2_pt*ph
r2h_h = 0.
r2h_r = 0.
c
a(1,1) = r1h_th
a(1,2) = r1h_ph
a(2,1) = r2h_th
a(2,2) = r2h_ph
c
detinv = 1.0 / (a(1,1)*a(2,2) - a(1,2)*a(2,1))
aikh(1,1) = a(2,2)*detinv
aih(2,2) = a(1,1)*detinv
aih(1,2) = -a(1,2)*detinv
aih(2,1) = -a(2,1)*detinv
c
dth = -(aih(1,1)*r1h + aih(1,2)*r2h)
dph = -(aih(2,1)*r1h + aih(2,2)*r2h)
c
c
ph = ph + dph
c
th = th + dth
c

c---- set and linearize new residuals: r1r = dr1/dr = 0, r2r = dr2/dr = 0

pr = p_r
tr = t_r
c
r1r = r1_p*pr + r1_t*tr + r1_r
r1r_pr = r1_p
r1r_tr = r1_t
\[
\begin{align*}
\text{rir}_p &= r_{1p} * pr + r_{1t} * tr + r_{1r} \\
\text{rir}_t &= r_{1t} * pr + r_{1r} * tr + r_{1t} \\
\text{rir}_r &= r_{1r} * pr + r_{1t} * tr + r_{1r} \\
\text{rir}_h &= 0.
\end{align*}
\]

\[
\begin{align*}
\text{r2r} &= -tm_1 * tr - tm_1 * pr - tm_2 * tr - tm_2 * pr \\
\text{r2r}_p &= -tm_1 \\
\text{r2r}_tr &= -tm_1 \\
\text{r2r}_p &= -tm_1 * tr - tm_1 * pr - tm_2 * pr \\
\text{r2r}_t &= -tm_1 * tr - tm_1 * pr - tm_2 * pr \\
\text{r2r}_h &= 0. \\
\text{r2r}_r &= 0.
\end{align*}
\]

\[
\begin{align*}
a(1,1) &= \text{rir}_tr \\
a(1,2) &= \text{rir}_pr \\
a(2,1) &= \text{r2r}_tr \\
a(2,2) &= \text{r2r}_pr \\
\text{detinv} &= 1.0 / (a(1,1) * a(2,2) - a(1,2) * a(2,1)) \\
\text{air}(1,1) &= a(2,2) * \text{detinv} \\
\text{air}(2,2) &= a(1,1) * \text{detinv} \\
\text{air}(1,2) &= -a(1,2) * \text{detinv} \\
\text{air}(2,1) &= -a(2,1) * \text{detinv}
\end{align*}
\]

\[
\begin{align*}
\text{dtr} &= -(\text{air}(1,1) * \text{rir} + \text{air}(1,2) * \text{r2r}) \\
\text{dpr} &= -(\text{air}(2,1) * \text{rir} + \text{air}(2,2) * \text{r2r})
\end{align*}
\]

\[
\begin{align*}
\text{pr} &= \text{pr} + \text{dpr} \\
\text{tr} &= \text{tr} + \text{dtr}
\end{align*}
\]

\[
\begin{align*}
\text{---- calculate responses in } \frac{dt}{dh} \text{ and } \frac{dp}{dh} \text{ to unit h perturbation} \\
\text{dr1h} &= \text{rir}_h + \text{rir}_p * ph + \text{rir}_t * th \\
\text{dr2h} &= \text{r2r}_h + \text{r2r}_p * ph + \text{r2r}_t * th \\
\end{align*}
\]

\[
\begin{align*}
\text{dr1r} &= \text{rir}_h + \text{rir}_p * ph + \text{rir}_t * th \\
\text{dr2r} &= \text{r2r}_h + \text{r2r}_p * ph + \text{r2r}_t * th \\
\end{align*}
\]

\[
\begin{align*}
\text{dth} &= -(\text{air}(1,1) * \text{dr1h} + \text{air}(1,2) * \text{dr2h}) \\
\text{dph} &= -(\text{air}(2,1) * \text{dr1h} + \text{air}(2,2) * \text{dr2h}) \\
\text{thh} &= \text{dth} \\
\text{phh} &= \text{dph}
\end{align*}
\]

\[
\begin{align*}
\text{dth} &= -(\text{air}(1,1) * \text{dr1r} + \text{air}(1,2) * \text{dr2r}) \\
\text{dph} &= -(\text{air}(2,1) * \text{dr1r} + \text{air}(2,2) * \text{dr2r}) \\
\text{thr} &= \text{dth} \\
\text{phr} &= \text{dph}
\end{align*}
\]

\[
\begin{align*}
\text{---- calculate responses in } \frac{dt}{dh} \text{ and } \frac{dp}{dh} \text{ to unit r perturbation} \\
\text{dr1h} &= \text{rir}_h * r + \text{rir}_p * pr + \text{rir}_t * tr \\
\text{dr2h} &= \text{r2r}_h * r + \text{r2r}_p * pr + \text{r2r}_t * tr
\end{align*}
\]
\[
dr _r = r r _r + r r _p r + r r _t \cdot t
\]
\[
dr _{r} = r 2 r _r + r 2 r _p r + r 2 r _t \cdot t
\]
\[
dth = - (a i h(1,1) \cdot d r _{h} + a i h(1,2) \cdot d r _{h})
\]
\[
dph = - (a i h(2,1) \cdot d r _{h} + a i h(2,2) \cdot d r _{h})
\]
\[
tr _h = dth
\]
\[
pr _h = dph
\]
\[
dth = - (a i h(1,1) \cdot d r _r + a i h(1,2) \cdot d r _r)
\]
\[
dph = - (a i h(2,1) \cdot d r _r + a i h(2,2) \cdot d r _r)
\]
\[
tr _r = dth
\]
\[
prr = dph
\]

---

set final first and second derivatives wrt (r,h)

\[
p _r = pr
\]
\[
t _r = tr
\]
\[
p _h = ph
\]
\[
t _h = th
\]
\[
p _{h h} = phh
\]
\[
t _{h h} = thh
\]
\[
p _{r r} = prr
\]
\[
t _{r r} = trr
\]
\[
p _{r h} = .5 * (prh + phr)
\]
\[
t _{r h} = .5 * (trh + thr)
\]

return

end

subroutine nonstag(h0, rho, q, p0, p0_r, p0_q, r0, r0_r, r0_q)

Calculates stagnation pressure and density for specified stagnation enthalpy, density, and speed.

Input:

h0 stagnation enthalpy
rho density
q speed

Output:

p0 stagnation pressure
p0_r dp0/dr
p0_q dp0/dq
r0 stagnation density
r0_r dr0/dr
r0_q dr0/dq

implicit real*4 (a-h,m,o-z)
dimension a(2,2), al(2,2), b(2,2)
real*4 h_p, h_t
common /nongas/
& alf, bta, pi, tau, z0
common /nonfit/
& c2, c1, c0

data eps /5.0E-6/

z(pp,tt) = 1. + pp*pi*phi (1./(tau*tt))
z_p(pp,tt) = pi*phi (1./(tau*tt))
z_t(pp,tt) = pp*pi*phid(1./(tau*tt)) / (-tau*tt**2)

h = h0 - .5*q**2
h_q = - q

h_h0 = 1.0

r = rho

set input pressure and temperature and derivatives
call ngaspt(h,r,p,p_r,p_h,p_rr,p_hh,p_rh,
& t,t_r,t_h,t_rr,t_hh,t_rh)

set entropy & and derivatives wrt p,t

ttc = 1./(tau*t)
ttc_t = -1./(tau*t**2)
ttc_tt = 2./(tau*tt**3)

ph = phi(ttc)
phd = phid(ttc)
phdd = phidd(ttc)
phddd = phiddd(ttc)

ph_t = phd * ttc_t
phd_t = phdd * ttc_t
phdd_t = phddd * ttc_t

s = alf*log(t) + 2.0*alf*bta*t
& - p*pi*( t*phd * ttc_t + ph ) - log(p)
s_p = - pi*( t*phd * ttc_t + ph ) - 1.0/p
s_t = alf/t + 2.0*alf*bta
& - p*pi( phd * ttc_t + ph_t
& + t*phd * ttc_t
& + t*phd * ttc_tt )

initial guess for p0,t0 from imperfect gas

if(bta.eq.0.0) then
  t0 = h0/alf
else
  t0 = (-1.0 + sqrt(1.0 + 4.0*bta*h0/alf)) / (2.0*bta)
endif

p0 = p * exp(-alf*log(t) + alf*2.0*bta*(1.0-t))

t0 = t
p0 = p
c------ Newton loop to converge on correct p0,t0
    itcon = 15
    do 100 iter=1, itcon
      
      ttc    = 1./tau*t0
      ttc_t0 = -1./tau*t0**2
      ttc_tt0 = 2./tau*t0**3
      
      ph    = phi(ttc)
      phd   = phid(ttc)
      phdd  = phidd(ttc)
      
      ph_t0  = phd * ttc_t0
      phd_t0 = phdd * ttc_t0
      phdd_t0 = phidd * ttc_t0
      
      c------ enthalpy residual
      res1  = (alf*(t0 + bta*t0**2) + p0*pi/tau*phd )/z0  -  h0
          r1_p0 = (  pi/tau*phd )/z0
          r1_t0 = (alf*(1.0+ bta*t0*2.) + p0*pi/tau*phd_t0)/z0
      
      c------ entropy residual
      res2 = alf*log(t0) + 2.0*alf*bta*t0
      & - p0*pi*( t0*phd *ttc_t0 + ph ) - log(p0) - s
      r2_p0 = - pi*( t0*phd *ttc_t0 + ph ) - 1.0/p0
      r2_t0 = alf/t0 + 2.0*alf*bta
            & - p0*pi*(  phd *ttc_t0 + ph_t0
            &       + t0*phd_t0*ttc_t0
            &       + t0*phd *ttc_tt0 )
      
      c------ setup and invert Jacobian matrix
      a(1,1) = r1_t0
      a(1,2) = r1_p0
      a(2,1) = r2_t0
      a(2,2) = r2_p0
      
      detinv = 1.0 / (a(1,1)*a(2,2) - a(1,2)*a(2,1))
      ai(1,1) = a(2,2)*detinv
      ai(2,2) = a(1,1)*detinv
      ai(1,2) = -a(1,2)*detinv
      ai(2,1) = -a(2,1)*detinv
      
      c------ set Newton variables
      dt = -(ai(1,1)*res1 + ai(1,2)*res2)
      dp = -(ai(2,1)*res1 + ai(2,2)*res2)
      
      rlx = 1.0
      if(rlx*dp .gt. 2.5*p0) rlx = 2.5*p0/dp
      if(rlx*dp .lt.  0.8*p0) rlx = 0.8*p0/dp
      if(rlx*dt .gt. 2.5*t0) rlx = 2.5*t0/dt
      if(rlx*dt .lt.  0.8*t0) rlx = 0.8*t0/dt
      
      c------ update variables

37
p0 = p0 + rlx*dp
t0 = t0 + rlx*dt

c

---- convergence check
if(abs(dp/p0) .le. eps .and. abs(dt/t0) .le. eps) go to 2

100 continue

write(*,*) 'NONSTAG: Convergence failure.'
write(*,*) 'dp dT :', dp, dt
write(*,*) 'p0 T0 h r:', p0, t0, h, r

2 continue

c

---- set residual derivatives wrt (s,h0)
  r1_s = 0.
  r2_s = -1.0
  r1_h = -1.0
  r2_h = 0.

c

b(1,1) = r1_s
b(1,2) = r1_h
b(2,1) = r2_s
b(2,2) = r2_h

c

---- set (t0,p0) derivatives wrt (s,h0)
  t0_s = -(ai(1,1)*b(1,1) + ai(1,2)*b(2,1))
  p0_s = -(ai(2,1)*b(1,1) + ai(2,2)*b(2,1))

c

---- convert derivatives wrt (s,h0) to wrt (p,t,h0)
  t0_t = t0_s*s_t
  t0_p = t0_s*s_p
  p0_t = p0_s*s_t
  p0_p = p0_s*s_p

c

---- set stagnation density r0 and derivatives wrt (p0,t0)
  zz = z(p0,t0)
  zz_p = z_p(p0,t0)
  zz_t = z_t(p0,t0)

r0 = z0/zz  * p0/t0
r0_z = -z0/zz**2  * p0/t0

r0_p0 = r0_z*zz_p + z0/(zz*zz_t)

r0_t0 = r0_z*zz_t - z0*p0/(zz*zz**2)

c

---- convert derivatives from wrt (p0,t0) to wrt (p,t,h0)
  r0_p = r0_p0*p0_p + r0_t0*t0_p
  r0_t = r0_p0*p0_t + r0_t0*t0_t
  r0_h0 = r0_p0*p0_h0 + r0_t0*t0_h0

c
c---- convert derivatives from wrt (p, t) to wrt (r, q, h0)

    r0_r = r0_p*p_r + r0_t*t_r
    r0_q = (r0_p*p_h + r0_t*t_h)*h_q
    p0_r = p0_p*p_r + p0_t*t_r
    p0_q = (p0_p*p_h + p0_t*t_h)*h_q

    r0_h0 = (r0_p*p_h + r0_t*t_h)*h_h0 + r0_h0
    p0_h0 = (p0_p*p_h + p0_t*t_h)*h_h0 + p0_h0

    return
    end

real*4 function phi(ttc)
implicit real*4(a-h,m,o-z)

  Returns function phi used in non-ideality parameter
  Z = 1 + pi*phi(ttc)

  common /nonfit/
    &    c2, c1, c0

  phi = c2*ttc**2 + c1*ttc + c0

  return
  end

real*4 function phid(ttc)
implicit real*4(a-h,m,o-z)
common /nonfit/
    &    c2, c1, c0

  phid = 2.*c2*ttc + c1

  return
  end

real*4 function phidd(ttc)
implicit real*4(a-h,m,o-z)
common /nonfit/
    &    c2, c1, c0

  phidd = 2.*c2

  return
  end

real*4 function phidd(ttc)
implicit real*4(a-h,m,o-z)
common /nonfit/
    &    c2, c1, c0
 subroutine hgent(h0,r,q,s)
  common /nongas/
    &   alf, bta, pi, tau, z0
  common /nonfit/
    &   c2, c1, c0
  h = h0 - .5*q**2

  ttc = 1./(tau*t)
  ttc_t = -1./(tau*t**2)
  ph = phi(ttc)
  phd = phid(ttc)
  s = alf*log(t) + 2.0*alf*bta*t
     - p*pi*(t*phd*ttc_t + ph) - log(p)

  return
end

 subroutine nongamv(h0,r,q,gam,gam_r,gam_q)
  common /nongas/
    &   alf, bta, pi, tau, z0
  common /nonfit/
    &   c2, c1, c0
  h = h0 - 0.5*q**2
  h_q = -q

  asq = p_r / (1. - p_h/r)
\[
\begin{align*}
\text{asq}_r &= \frac{p_{rr}}{(1. - p_h/r)} \\
&\quad - \frac{p_r}{(1. - p_h/r)^2} \ast (p_h/r^2 - p_{rh}/r) \\
\text{asq}_h &= \frac{p_{rh}}{(1. - p_h/r)} \\
&\quad + \frac{p_r}{(1. - p_h/r)^2} \ast p_{hh}/r
\end{align*}
\]

\[
\begin{align*}
\text{ttc} &= 1./\text{(tau} \ast t) \\
\text{ttc}_t &= -1./\text{(tau} \ast t \ast 2) \\
\text{ttc}_tt &= 2./\text{(tau} \ast t \ast 3)
\end{align*}
\]

\[
\begin{align*}
\text{ph} &= \text{phi}(\text{ttc}) \\
\text{phd} &= \text{phid}(\text{ttc}) \\
\text{phdd} &= \text{phidd}(\text{ttc}) \\
\text{phddd} &= \text{phidd}(\text{ttc})
\end{align*}
\]

\[
\begin{align*}
z &= 1. + p \ast \pi \ast \text{ph} \\
z_p &= p \ast \pi \ast \text{ph} \\
z_t &= p \ast \pi \ast \text{phd} \ast \text{ttc}_t
\end{align*}
\]

\[
\begin{align*}
\text{cp} &= (\alpha \ast (1.0 + 2.0 \ast \text{bta} \ast t) \\
&\quad + p \ast \pi / \text{tau} \ast \text{phdd} \ast \text{ttc}_t) / z_0 \\
\text{cp}_p &= (p \ast \pi / \text{tau} \ast \text{phdd} \ast \text{ttc}_t) / z_0 \\
\text{cp}_t &= (\alpha \ast (2.0 \ast \text{bta} \\
&\quad + p \ast \pi / \text{tau} \ast \text{phdd} \ast \text{ttc}_t) / z_0
\end{align*}
\]

\[
\begin{align*}
\text{zet} &= h / (\text{cp} \ast t) \ast (1.0 - p \ast \pi / (\text{tau} \ast \text{phdd} / z) \ast z_0 \\
\text{zet}_h &= 1.0 / (\text{cp} \ast t) \ast (1.0 - p \ast \pi / (\text{tau} \ast \text{phdd} / z) \ast z_0 \\
\text{zet}_p &= h / (\text{cp} \ast t) \ast ( - \pi / (\text{tau} \ast \text{phdd} / z) \\
&\quad - p \ast \pi / (\text{tau} \ast \text{phdd} / z \ast (-z_p / z)) \ast z_0 \\
&\quad - (zet / cp) \ast cp_p \\
\text{zet}_t &= h / (cp \ast t) \ast ( - p \ast \pi / (\text{tau} \ast \text{phdd} / z \ast (-z_t / z - 1.0 / t) \\
&\quad - p \ast \pi / (\text{tau} \ast \text{phdd} \ast \text{ttc}_t / z) \ast z_0 \\
&\quad - (zet / cp) \ast cp_t - (zet / t)
\end{align*}
\]

\[
\begin{align*}
\text{gam} &= \text{asq} / (h \ast \text{zet}) + 1.0 \\
\text{gam}_r &= \text{asq} / (h \ast \text{zet}) \\
\text{gam}_h &= \text{asq} / (h \ast \text{zet}) \ast (-zet_h / zet - 1.0 / h) + \text{asq} / (h \ast \text{zet}) \\
\text{gam}_p &= \text{asq} / (h \ast \text{zet}) \ast (-zet_p / zet) \\
\text{gam}_t &= \text{asq} / (h \ast \text{zet}) \ast (-zet_t / zet)
\end{align*}
\]

\[
\begin{align*}
\text{gam}_h &= \text{gam}_p \ast p_h + \text{gam}_t \ast t_h + \text{gam}_h \\
\text{gam}_r &= \text{gam}_p \ast p_r + \text{gam}_t \ast t_r + \text{gam}_r
\end{align*}
\]

\[
\begin{align*}
\text{gam}_q &= \text{gam}_h \ast h \ast q
\end{align*}
\]

return
end

subroutine sonic(h0,p0,r0, q,p,r)
\begin{center}
\text{calculates sonic quantities q,p,r from specified sonic quantities h0,p0,r0}
\end{center}
! implicit real (a)
! data eps / 1.0e-5 /
!
!--- initialize with perfect gas
! gam = r0*h0 / (r0*h0 - p0)
! gm1 = gam - 1.0
!
! q = sqrt(2.0*h0/(2.0/gm1 + 1.0))
!
! trat = 1.0 + 0.5*gm1
! p = p0*trat**(gam/gm1)
! r = r0*trat**(1.0/gm1)
!
!--- converge on non-ideal values by forcing Ma^2 = 1, and pstag = p0
! do 10 iters=1, 15
! call nideal(h0,r,q, p ,p_r ,p_q, 
! & msq,msq_r,msq_q )
! call nonstag(h0,r,q, pstag,pstag_r,pstag_q, 
! & rstag,rstag_r,rstag_q )
! res1 = msq - 1.0
! a11 = msq_r
! a12 = msq_q
!
! res2 = pstag - p0
! a21 = pstag_r
! a22 = pstag_q
!
! detinv = 1.0/(a11*a22 - a12*a21)
! dr = -(res1*a22 - a12*res2)*detinv
! dq = -(a11*res2 - res1*a21)*detinv
!
! dp = p_r*dr + p_q*dq
!
! rlx = 1.0
! if(rlx*dr .gt. 1.6*r) rlx = 1.6*r/dr
! if(rlx*dr .lt. -.6*r) rlx = -.6*r/dr
! if(rlx*dq .gt. 1.6*q) rlx = 1.6*q/dq
! if(rlx*dq .lt. -.6*q) rlx = -.6*q/dq
!
! r = r + rlx*dr
! q = q + rlx*dq
! p = p + rlx*dp
!
! dmax = amax1( abs(dr)/r , abs(dq)/q )
!
! if(dmax .lt. eps) go to 11
!
10 continue
! write(*,*), 'sonic: convergence failed. dmax = ', dmax
11 continue
!
return
!
end ! sonic

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Bibliography


Appendix B
High-Order Airfoil Farfield Boundary Conditions
for Ideal and Non-Ideal Gas Flows

The steady flow around an airfoil away from shock wakes and viscous regions has constant entropy and total enthalpy, and hence is also irrotational. These properties hold whether the fluid is an ideal or a non-ideal gas. The flow can then still be described by the velocity potential \( \Phi \) or the perturbation potential \( \phi \). Assuming the freestream is aligned with the \( z \)-axis, the following relations are obtained.

\[
\Phi = q_\infty (x + \phi) \quad (1)
\]
\[
\nabla \Phi \equiv \vec{q} = q_\infty [(1 + \phi_x)i + \phi_y j] \quad (2)
\]
\[
q^2 \equiv |\vec{q}|^2 = q_\infty^2 [(1 + \phi_x)^2 + \phi_y^2] \quad (3)
\]
\[
\frac{1}{2} \nabla (q^2) = q \nabla q = q_\infty^2 [(\phi_{xx} + \phi_x \phi_{xx} + \phi_y \phi_{xy})i + (\phi_{xy} + \phi_x \phi_{xy} + \phi_y \phi_{yy})j] \quad (4)
\]

The governing flow equation is:

\[
\nabla \cdot (\rho \nabla \Phi) = 0 \quad (5)
\]
or
\[
\nabla^2 \Phi = -\frac{\nabla \rho}{\rho} \cdot \nabla \Phi \quad (6)
\]

In isentropic flow \( (s = \text{constant}) \), \( \rho = \rho(p) \), so

\[
\nabla \rho = \left. \frac{dp}{dp} \right|_s \nabla p = \frac{\rho}{a^2} q \nabla q \quad (7)
\]

and hence

\[
\nabla^2 \Phi = \frac{1}{a^2} p q \nabla q \cdot \nabla \Phi \quad (8)
\]
\[
a^2 \nabla^2 \phi = q \nabla q \cdot [(1 + \phi_x)i + \phi_y j] \quad (9)
\]

where \( a \) is the speed of sound. In isentropic, adiabatic flow, the speed of sound is uniquely related to the speed: \( a = a(q) \). For a perfect gas, \( a(q) \) is given by

\[
a^2 = a^2_\infty - \frac{\gamma - 1}{2} (q^2 - q^2_\infty) \quad (10)
\]

while for an imperfect and/or non-ideal gas it is necessary here to linearize \( a(q) \) about the freestream conditions.

\[
a^2 \simeq a^2_\infty + \left. \frac{d(a^2_\infty)}{d(q^2_\infty)} \right|_s (q^2 - q^2_\infty) \quad (11)
\]

It is convenient to define an "equivalent" ratio of specific heats \( \gamma' \) for the non-ideal gas as

\[
\gamma' \equiv 1 - 2 \left. \frac{d(a^2_\infty)}{d(q^2_\infty)} \right|_s \quad (12)
\]
so that the \( a(q) \) relation for the non-ideal gas can be compactly written as

\[
a^2 \approx a_\infty^2 - \frac{\gamma' - 1}{2} \left( q^2 - q_\infty^2 \right)
\]  

(13)

For a perfect gas, this reverts to the exact form (10) since in this case \( \gamma' = \gamma \). It is interesting to note that \( \gamma' \) can easily be less than unity for heavy gases such as sulfur hexafluoride, while invariably \( \gamma > 1 \) for perfect gases.

Substituting for \( a^2 \), \( q^2 \), and \( q \nabla q \) in equation (9), we obtain

\[
\left[ a_\infty^2 - \frac{\gamma' - 1}{2} q_\infty^2 \left( 2\phi_z + \phi_z^2 + \phi_y^2 \right) \right] \left[ \phi_{xz} + \phi_{yy} \right] = q_\infty^2 \left[ (1 + \phi_x) \left( \phi_{xz} + \phi_z \phi_{zz} + \phi_y \phi_{zy} \right) + \phi_y \left( \phi_{zy} + \phi_z \phi_{yy} + \phi_y \phi_{yy} \right) \right]
\]

(14)

\[
\left[ 1 - \frac{\gamma' - 1}{2} M_\infty^2 \phi_z \right] \left[ \phi_{xz} + \phi_{yy} \right] = M_\infty^2 \left[ \phi_{xz} + 2\phi_z \phi_{zz} + 2\phi_y \phi_{zy} \right] + \mathcal{O} \left( \phi^3 \right)
\]

(15)

\[
(1 - M_\infty^2) \phi_{xz} + \phi_{yy} = M_\infty^2 \left[ (\gamma' + 1) \phi_z \phi_{xz} + (\gamma' - 1) \phi_z \phi_{yy} + 2\phi_y \phi_{zy} \right] + \mathcal{O} \left( \phi^3 \right)
\]

(16)

where \( M_\infty = q_\infty / a_\infty \) is the freestream Mach number.

Equation (16) is the 2D second-order Prandtl-Glauert equation which governs small-perturbation non-ideal compressible potential flows. It has the same form as the equation for a perfect ideal gas as derived in references [4] and [5], except that the usual ratio of specific heats \( \gamma \) is replaced by the “equivalent” value \( \gamma' \) defined by equation (12). Wagner and Schmidt [1] have considered the first-order version of equation (16) using \( \gamma' \) in lieu of \( \gamma \).

In terms of the Prandtl-Glauert coordinates

\[
\tilde{x} = x / \beta
\]

(17)

\[
\tilde{y} = y
\]

(18)

\[
\tilde{r}^2 = \tilde{x}^2 + \tilde{y}^2
\]

(19)

\[
\theta = \arctan \frac{\tilde{y}}{\tilde{x}}
\]

(20)

where \( \beta = \sqrt{1 - M_\infty^2} \), the general solution to equation (16) is

\[
\phi = \frac{-\Gamma}{2\pi} \theta + \frac{\Sigma}{2\pi} \ln \tilde{r}
\]

\[
+ \frac{D_x \cos \theta}{2\pi} \tilde{r} + \frac{D_y \sin \theta}{2\pi} \tilde{r}
\]

\[
+ \left( \frac{\Gamma M_\infty}{2\pi} \right)^2 \left[ k_1 \ln \frac{\tilde{r}}{\tilde{x}} - k_2 \cos 3\theta \right]
\]

(21)

where

\[
k_1 = \frac{1}{4} \left( \frac{\gamma' + 1}{\beta^3} + \frac{4 - \gamma'}{\beta} \right) \quad k_2 = \frac{1}{16} \left( \frac{\gamma' + 1}{\beta^3} + \frac{\gamma' - 1}{\beta} \right)
\]

(22)

Terms of order \( 1/\tilde{r}^2 \) and above have been discarded.
In a flow solver, the circulation \( \Gamma \) can be determined either directly from the lift per unit span \( L' \) (Euler or Navier-Stokes code),
\[
\Gamma = \frac{L'}{\rho_\infty q_\infty^2}
\]  
(23)
or indirectly by specifying a Kutta condition (potential solver or MSES). The source strength \( \Sigma \) can be determined from the total profile drag per unit span \( D' \), or from the asymptotic mass defect behind the airfoil including the shock wake.
\[
\Sigma = \frac{D'}{\rho_\infty q_\infty^2}
\]  
(24)
In the case of a potential solver, \( D' \) should not include the wave drag since there is no shock wake (unless an entropy correction scheme is employed). Note that \( \Gamma \) and \( \Sigma \) here have units of length since \( \phi \) in (1) corresponds to a unit freestream speed.

Cole and Cook [5] give explicit expressions for the doublet coefficients \( D_x \) and \( D_y \) in terms of field integrals over the domain. Unfortunately, these expressions are unwieldy and for a non-ideal gas would be rather expensive. A simpler and economical approach is to iteratively update \( D_x \) and \( D_y \) by minimizing the mismatch between \( \nabla \Phi \) and the velocity \( \vec{q}_{\text{solution}} \) from the flow solver on the outer boundary. The approach taken in reference [4], for example, is to minimize the integral
\[
I = \frac{1}{2} \int |\nabla \Phi \times \vec{q}_{\text{solution}}|^2 \, dx
\]  
(25)
taken over the outermost streamlines. The doublet terms in the farfield expansion (21) decay faster than the others, and so can be neglected for sufficiently distant outer boundaries. However, retaining them greatly reduces the sensitivity of the solution to domain size, especially for transonic flows [6].

With its term coefficients defined, equation (21) gives a very accurate representation of the perturbation potential \( \phi \) away from the airfoil. The gradient of equation (21) accurately gives the total velocity \( \vec{q} \) via relation (2). Either \( \phi \), \( \vec{q} \), or an appropriate derived quantity may then be imposed at the outer domain boundary as a high-order boundary condition. A potential solver would typically impose \( \phi \) or \( \partial \phi / \partial n \), whereas an Euler or Navier-Stokes solver would typically impose the flow angle at the inflow and pressure at the outflow, both being determined from \( \nabla \Phi \).
Appendix C
Shape Parameter Relations
for Ideal and Non-Ideal Gas Flows

The major influence of compressibility on boundary layer behavior is a non-uniform density profile, which alters the layer's response to pressure gradients. In an integral scheme for adiabatic flows, this effect is mostly captured by the correlation between shape parameter $H$, the kinematic shape parameter $H_k$, and the edge Mach number $M_e$. The shape parameters are defined as

$$H \equiv \frac{\int (1 - RU) \, dy}{\int (1 - U) \, dy} \quad H_k \equiv \frac{\int (1 - U) \, dy}{\int (1 - U) U \, dy}$$

(26)

where $U(y)$ and $R(y)$ are the velocity and density profiles.

$$U = \frac{u}{u_e} \quad R = \frac{\rho}{\rho_e}$$

(27)

Since the velocity profile $U(y)$ and hence $H_k$ are only weakly affected by compressibility, reduction of the density profile $R(y)$ near the wall due to adiabatic heating will increase $H$ as can be seen from its definition (26). In turn, the von-Karman integral momentum equation

$$\frac{d\theta}{dz} = \frac{C_f}{2} - (2 + H - M_e^2) \frac{\theta}{u_e} \frac{du_e}{dz}$$

(28)

shows that an increase in $H$ will increase the momentum thickness growth rate $d\theta/dz$ for a given adverse pressure gradient. The integral boundary layer formulation in MSES (and its precursor ISES [4]) employs a correlation of the form $H_k(H, M_e)$ for air. This is re-derived for the non-ideal gas model as follows.

As developed in Appendix A, the state equation of a non-ideal gas can be written as

$$\frac{p}{\rho R T} = Z(p, T)$$

(29)

while the corresponding caloric equation in differential form is

$$dh = \varepsilon_p(T) \, dT + d[pF(T)] \simeq \varepsilon_p(T) \, dT + pF'(T) \, dT = c_p(p, T) \, dT$$

(30)

where the approximation is made on the basis that $dp \simeq 0$ across a boundary layer. Linearizing the caloric equation across the boundary layer we have

$$h - h_e = c_p(T - T_e)$$

(31)

$$\frac{T_e}{T} - 1 = \left(\frac{h_e}{h} - 1\right) \frac{h}{c_p T_e}$$

$$\simeq \left(\frac{h_e}{h} - 1\right) \frac{h_e}{c_{pe} T_e}$$

(32)

The non-ideality factor $Z$ for most non-ideal gases has the form

$$Z(p, T) = 1 + \frac{p}{p_c} \phi(T_e/T)$$

(33)
where $p_c$ and $T_c$ are the critical pressure and temperature. This can likewise be linearized about the edge conditions as follows.

$$Z - Z_e = \frac{p_c}{p_c} \phi_e \left( \frac{T}{T_c} - \frac{T}{T_e} \right)$$

$$\frac{Z_e}{Z} = 1 - \frac{p_c}{p_c} \frac{T_e}{T_e} \left( \frac{T_e}{T} - 1 \right) \frac{\phi_e}{Z}$$

Combining this with equation (32), we have

$$\frac{Z_e}{Z} = 1 - \frac{p_c}{p_c} \frac{T_e}{T_e} \left( \frac{h_e}{h} - 1 \right) \frac{h_e}{c_p T_e Z_e} \phi_e .$$

Using the equation of state (29), the density profile is then related to the $T$ and $Z$ profiles as

$$R = \frac{\rho}{\rho_e} = \frac{T_e Z_e p}{T Z p_e} = \frac{T_e Z_e}{T Z}$$

with the usual boundary layer approximation $p \approx p_e$ being made. Using relations (32) and (36), the density profile can be written in terms of the enthalpy profile alone.

$$R = \left[ 1 + \left( \frac{h_e}{h} - 1 \right) \frac{h_e}{c_p T_e} \right] \left[ 1 - \frac{p_c}{p_c} \frac{T_e}{T_e} \left( \frac{h_e}{h} - 1 \right) \frac{h_e}{c_p T_e Z_e} \phi_e \right]$$

$$= 1 + \left( \frac{h_e}{h} - 1 \right) \frac{h_e}{c_p T_e} \left( 1 - \frac{p_c}{p_c} \frac{T_e}{T_e} \phi_e \right) + \mathcal{O} \left( \frac{h_e}{h} \right)^2$$

$$R \approx 1 + \left( \frac{h_e}{h} - 1 \right) \zeta$$

where

$$\zeta = \frac{h_e}{c_p T_e} \left( 1 - \frac{p_c}{p_c} \frac{T_e}{T_e} \phi_e \right)$$

For turbulent adiabatic boundary layer flows, it is reasonable to assume a constant stagnation enthalpy across the layer, although this is strictly true only for a turbulent Prandtl number of unity. Since the turbulent diffusion mechanisms of momentum and heat are essentially the same in a gas (convection by eddies), turbulent Prandtl numbers are typically close to unity. Hence, the assumption of constant stagnation enthalpy is reasonable. With $h_0$ denoting the stagnation enthalpy, the velocity and static enthalpy profiles are then related by

$$\frac{h_e}{h} = \frac{h_0 - u^2/2}{h_0 - u^2/2} = \frac{1 - \frac{u^2}{2h_0}}{1 - \frac{u^2}{2h_0} U^2}$$

$$\frac{h_e}{h} - 1 = \frac{u^2}{2h_0} (U^2 - 1) \frac{1}{1 - \frac{u^2}{2h_0} U^2}$$

and the density and velocity profiles are then related by

$$R = 1 + \frac{\frac{u^2}{2h_0} (U^2 - 1)}{1 - \frac{u^2}{2h_0} U^2} \zeta .$$
Since $u_2^2/h_0$ and $\zeta$ are both functions of the edge Mach number $M_e$, the density profile (44) implicitly defines $H_k$ in terms of $H$ and $M_e$. To obtain this relation in closed form, it is necessary to assume a small-defect profile

$$U = 1 - \epsilon \quad ; \quad \epsilon \ll 1$$

(45)

so that the density profile can be approximated by

$$R = 1 + \frac{u_2^2}{2h_0} \left( \frac{-2\epsilon}{1 - \frac{u_2^2}{2h_0}} \zeta \right) + \mathcal{O}(\epsilon^2)$$

(46)

$$R = 1 - (\gamma_v - 1)M_e^2 \epsilon \zeta$$

(47)

with the convenient "viscous" equivalent ratio of specific heats $\gamma_v$ defined by

$$\frac{\gamma_v - 1}{2}M_e^2 \zeta = \frac{u_2^2}{2h_0} \frac{1}{1 - \frac{u_2^2}{2h_0}}$$

(48)

$$\gamma_v = 1 + \frac{a_e^2}{h_0 - u_2^2/2 \zeta} \frac{1}{1 - \epsilon}$$

(49)

with $a_e$ being the speed of sound at the boundary layer edge.

The shape parameter $H$ now becomes

$$H = \frac{\int \{ 1 - [1 - (\gamma_v - 1)M_e^2 \epsilon] (1 - \epsilon) \} dy}{\int \{ \epsilon [1 - (\gamma_v - 1)M_e^2 \epsilon] (1 - \epsilon) \} dy}$$

$$= \frac{\int \epsilon dy + (\gamma_v - 1)M_e^2 \int \epsilon (1 - \epsilon) dy}{\int \epsilon (1 - \epsilon) dy - (\gamma_v - 1)M_e^2 \int \epsilon^2 (1 - \epsilon) dy}$$

$$= \frac{\int \epsilon dy}{\int \epsilon (1 - \epsilon) dy} + (\gamma_v - 1)M_e^2 + \mathcal{O}(\epsilon^2)$$

$$\approx H_k + (\gamma_v - 1)M_e^2$$

(50)

The required shape parameter correlation is therefore

$$H_k = H - (\gamma_v - 1)M_e^2.$$  

(51)

In the limiting case of a perfect gas, $\gamma_v = \gamma$. For $\gamma = 1.4$ (air), MSES presently uses Whitfield's correlation [7] in this case is

$$H_k = \frac{H - 0.29M_e^2}{1 + 0.113M_e^2}$$

$$= H - 0.4M_e^2 + \mathcal{O}(M_e^4)$$

(52)

(53)

which is seen to be consistent with the more general non-ideal gas result (51). Whitfield's particular form (52), however, is reportedly more accurate for Prandtl numbers somewhat less than unity.
where the total enthalpy profile is not quite uniform as was assumed here. It is therefore appropriate to put correlation (51) into Whitfield's form, while also incorporating the Prandtl number. The final shape parameter correlation is

\[ H_k(H, M_e) = \frac{H - Pr(\gamma_v - 1)M_e^2}{1 + (1-Pr)(\gamma_v - 1)M_e^2} \]  

(54)

which reduces to Whitfield's form for \( \gamma_v = 1.4, \zeta = 1, \) and \( Pr = 0.7, \) and to the non-ideal gas form (51) for \( Pr = 1 \) which was assumed in its derivation.

It noteworthy that for most heavy gases \( \gamma_v - 1 \) is considerably smaller than for air. For \( SF_6 \) with stagnation conditions at STP and \( M_e = 1, \) for example, \( \gamma_v - 1 = 0.17 \) for \( SF_6 \) and \( \gamma_v - 1 = \gamma - 1 = 0.4 \) for air. Hence, the influence of \( M_e \) in \( SF_6 \) is smaller, and \( H \) values near a shock in \( SF_6 \) will be smaller than those in air. The smaller \( H \) values in turn reduce the boundary layer's response to adverse pressure gradients as discussed above. The airfoil will therefore be more resistant to Mach drag-divergence in \( SF_6 \) than in air.

For simplicity, the implementation of the shape parameter correlation (54) in MSES assumes that \( \gamma_v \) is constant, being evaluated from (49) at sonic edge conditions: \( a_e = u_e = a^* , M_e = 1. \) Given the degree of approximation used in deriving (54), it is felt that neglecting the already weak dependence of \( \gamma_v \) on \( u_e \) is justified. Freezing \( \gamma_v \) at the sonic conditions is judged appropriate since its effect on \( H \) becomes significant only for \( M_e \) close to unity.