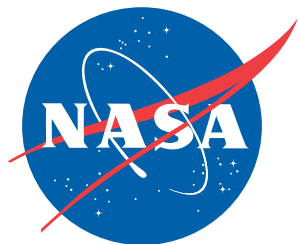


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NESC-RP-07-037



Reacting Multi-Species Gas Capability for USM3D Flow Solver

*Neal T. Frink and David M. Schuster/NESC
Langley Research Center, Hampton, Virginia*

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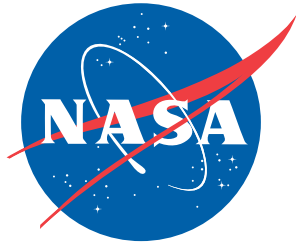
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Space Administration


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May 2012

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March 8, 2012

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Approval and Document Revision History

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Approved:	<i>Original Signature on File</i> <hr style="width: 80%; margin: 0 auto;"/> NESC Director	4/25/12 <hr style="width: 80%; margin: 0 auto;"/> Date
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Version	Description of Revision	Office of Primary Responsibility	Effective Date
1.0	Initial Release	Dr. Neal T. Frink, Senior Research Engineer, Langley Research Center	3/8/12



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Technical Assessment Report

1.0 Notification and Authorization

The NASA Engineering and Safety Center (NESC) approved this assessment on June 14, 2007. Dr. Neal Frink, Senior Research Engineer at Langley Research Center (LaRC), was selected to lead this assessment. The Phase I Assessment Plan was approved by the NESC Review Board (NRB) on July 12, 2007. The Phase II Assessment Plan was approved by the NRB on December 16, 2008.

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2.0 Signature Page

Submitted by:

Team Signature Page on File – 5/4/12

Dr. Neal T. Frink

Date

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Date

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Dr. Gary Cheng

Date

Dr. Roy P. Koomullil


Date

Signatories declare the findings, observations, and NESC recommendations compiled in the report are factually based from data extracted from Program/Project documents, contractor reports, and open literature, and/or generated from independently conducted tests, analyses, and inspections.

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3.0 Team List

Name	Discipline	Organization/Location
Core Team		
Neal Frink	Team Lead, Senior Research Engineer	LaRC
Dave Schuster	NASA Technical Fellow for Aerosciences	LaRC
Mohagna Pandya	USM3D Expert	LaRC
Gary Cheng	Investigator	University of Alabama at Birmingham/Mechanical Engineering
Roy Koomullil	Investigator	University of Alabama at Birmingham/Mechanical Engineering
Patricia Pahlavani	MTSO Program Analyst	LaRC
Administrative Support		
Christina Williams	Technical Writer	ATK, LaRC

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4.0 Executive Summary


The USM3D Navier-Stokes flow solver contributed heavily to the NASA Constellation Project (CxP) as a highly productive computational tool for generating the aerodynamic databases for the Ares I and V launch vehicles and Orion launch abort vehicle (LAV). At the peak of that effort, USM3D was consuming approximately 25 percent of the total available computer resources on the 10,000-processor NASA Advanced Supercomputing Columbia machine at the NASA Ames Research Center for these projects.

Some of the largest database uncertainties were associated with inadequate aerodynamic modeling of jet impingement. For example, the aerodynamic modeling uncertainties from the abort motor plume impingement on the LAV flight vehicle continually contributed to failure of the flight simulations, which elevated the risk to flight safety for launch abort. Similar uncertainties were present in the jet impingement from the Ares roll control system (RCS). There is a need to improve this deficiency through implementation of more physically correct models of the hot-gas jet flows. Efforts to resolve these uncertainties within any of the flow solvers used in the CxP have not been successful to date.

USM3D is currently limited to ideal-gas flows, which are not adequate for modeling the chemistry or temperature effects of hot-gas jet flows. This task was initiated to create an efficient implementation of multi-species gas and equilibrium chemistry into the USM3D code to improve its predictive capabilities for hot jet impingement effects. A finite-rate chemistry model was also pursued to improve future predictions of re-entry heating rates of planetary entry vehicles.

The effort was only partially successful as the investigators struggled with converting an existing flow solver with tightly embedded ideal-gas assumptions to a real-gas chemistry code. At this time, the implementation of the real-gas and multi-species transport equations has been verified on simple unit problems, but has not been validated against experimental data. Also, some numerical solution stability issues are yet to be resolved. The modules for the equilibrium and reacting chemistry were developed, but were not implemented because of the prior difficulties.

Work is continuing through the support of the Space Launch System (SLS) Aero Task Lead, Dr. John Blevins at NASA Marshall Space Flight Center, using the services of subject matter experts, including: Dr. Michael Applebaum, Dr. William Eppard, and Mr. Les Hall at CRM Solutions, Inc., in Huntsville, Alabama. Assessments are underway to determine the best path forward. The near-term goal is to resolve the numerical stability issues with the multi-species capability as soon as possible and commence application to Multi-Purpose Crew Vehicle (MPCV) launch abort and SLS RCS jet cases. The long-term goal is to implement and test the equilibrium and reacting-gas capability.

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5.0 Assessment Plan


The goal of this assessment was to implement and validate a simulation capability to handle real-gas effects in the USM3D code. This implementation was proposed as a three-step process:

1. Modification of governing equations to handle variable ratio of specific heats.
2. Addition of species transport equations to model the transport and mixing of multiple species in the computational domain.
3. Addition of capability for different species to react with each other and produce new species.

A detailed description of the USM3D code modifications, addition of new capabilities, and implementation model validation are described in the following sections.

6.0 Problem Description

The underlying physics associated with flow around a supersonic/hypersonic vehicle is complex, which involves an oblique/bow shock, air dissociation (or ionization), and large heat transfer. Accurate predictions of the aerothermodynamics of supersonic/hypersonic vehicles require efficient numerical models for resolving chemical reactions and modeling of transport of multiple species, and accurate estimation of heat transfer. The modeling of chemical reactions and species transport is also important in the numerical simulation of combustion. Challenges involved in the simulation of flows with chemical reactions are the stability and efficiency issues associated with the numerical methods. The stability of the numerical scheme for the species equation is hindered by disparity between the time scales for the mean flow and chemical reactions and the stiffness problem of the source terms. Various methods were developed to alleviate the stiffness problem and to efficiently solve a large set of species transport equations with momentum and energy equations. Since each method has its strength and weakness, the USM3D code needed to be analyzed with the assistance of the code developer to determine the numerical method most appropriate to efficiently and accurately solve the set of governing equations. This report describes the addition of the chemically-reacting flow capability into the USM3D code.

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7.0 Technical Approach

Section 14.1 provides the nomenclature definitions for equations used in the following sections.

7.1 Theoretical Formulation

Governing Equations

The governing equations for single-species real-gas flow can be expressed as:

$$\text{Continuity equation: } \frac{\partial \hat{\rho}}{\partial \hat{t}} + \hat{\nabla} \cdot (\hat{\rho} \vec{\hat{V}}) = 0 \quad (1)$$

$$\text{Momentum equation: } \frac{\partial (\hat{\rho} \vec{\hat{V}})}{\partial \hat{t}} + \hat{\nabla} \cdot (\hat{\rho} \vec{\hat{V}} \vec{\hat{V}}) = -\hat{\nabla} \hat{p} + \hat{\nabla} \cdot \vec{\hat{\tau}} \quad (2)$$

$$\text{Total energy equation: } \frac{\partial}{\partial \hat{t}} \hat{\rho} \hat{E} + \hat{\nabla} \cdot [\vec{\hat{V}} (\hat{\rho} \hat{E} + \hat{p})] = \hat{\nabla} \cdot (\hat{\kappa} \hat{\nabla} \hat{T}) + \hat{\nabla} \cdot (\vec{\hat{\tau}} \cdot \vec{\hat{V}}) + \hat{Q} \quad (3)$$


where $\hat{E} = \hat{e} + \frac{1}{2}(\hat{u}^2 + \hat{v}^2 + \hat{w}^2)$, and $\hat{\kappa}$ (thermal conductivity) = $\frac{\hat{C}_p \hat{\mu}}{\text{Pr}}$.

The set of governing equations is non-dimensionalized with a set of reference quantities as:

(ℓ_{ref} , ρ_{ref} , a_{ref} , T_{ref} , R_{ref} , γ_{ref} , and μ_{ref}), such as:

$$\begin{aligned} \nabla &= \hat{\nabla} \ell_{\text{ref}}; \quad \vec{V} = \frac{\vec{\hat{V}}}{a_{\text{ref}}}; \quad t = \frac{\hat{t}}{\ell_{\text{ref}}/a_{\text{ref}}}; \quad \rho = \frac{\hat{\rho}}{\rho_{\text{ref}}}; \quad p = \frac{\hat{p}}{\rho_{\text{ref}} a_{\text{ref}}^2}; \quad T = \frac{\hat{T}}{T_{\text{ref}}} \\ e &= \frac{\hat{e}}{a_{\text{ref}}^2}; \quad E = \frac{\hat{E}}{a_{\text{ref}}^2} = \frac{\hat{e}}{a_{\text{ref}}^2} + \frac{|\vec{\hat{V}}|^2}{2a_{\text{ref}}^2}; \quad \mu = \frac{\hat{\mu}}{\mu_{\text{ref}}}; \quad R = \frac{\hat{R}}{R_{\text{ref}}}; \quad C_p = \frac{\hat{C}_p}{R_{\text{ref}}}; \quad C_v = \frac{\hat{C}_v}{R_{\text{ref}}} \\ \gamma_{\text{ref}} &= \left(\frac{C_p}{C_v} \right)_{\text{ref}} = \frac{1}{1 - (R/C_p)_{\text{ref}}}; \quad a_{\text{ref}} = \sqrt{\gamma_{\text{ref}} R_{\text{ref}} T_{\text{ref}}}; \quad \kappa = \frac{\hat{\kappa}}{R_{\text{ref}} \mu_{\text{ref}}}; \quad \dot{Q} = \frac{\hat{Q}}{\rho_{\text{ref}} a_{\text{ref}}^3 / \ell_{\text{ref}}} \end{aligned} \quad (4)$$

The reference length scale (ℓ_{ref}) was read into the USM3D code through input based on the unit of the mesh coordinates. If the air at the sea level (1 atm and 300K) was taken as reference state, then the reference temperature (T_{ref}), pressure (p_{ref}), species mass fractions ($\alpha_{s,\text{ref}}$), the reference gas constant (R_{ref}), reference density (ρ_{ref}), reference specific heats ratio (γ_{ref}), reference speed of sound (a_{ref}), and reference viscosity (μ_{ref}) were determined automatically. The values of all flow variables and mesh coordinates were non-dimensionalized based on this set of reference quantities once they were read into the code. The solution of the flowfield was

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calculated based on the non-dimensionalized governing equation. The Sutherland law for air was used as:

$$\begin{aligned} \therefore \frac{\hat{\mu}}{\hat{\mu}_0} &= \left(\frac{\hat{T}}{\hat{T}_0} \right)^{1.5} \frac{\hat{T}_0 + S}{\hat{T} + S} \\ \Rightarrow \mu &= \frac{\hat{\mu}}{\mu_{\text{ref}}} = \frac{\hat{\mu}}{\hat{\mu}_0} \frac{\hat{\mu}_0}{\mu_{\text{ref}}} = \frac{\hat{\mu}_0}{\mu_{\text{ref}}} \left(\frac{\hat{T}}{\hat{T}_0} \right)^{1.5} \frac{\hat{T}_0 + S}{\hat{T} + S} = \frac{\hat{\mu}_0}{\mu_{\text{ref}}} \left(\frac{T}{T_0} \right)^{1.5} \frac{T_0 + S/T_{\text{ref}}}{T + S/T_{\text{ref}}} \end{aligned} \quad (5)$$

If $\hat{T}_0 = T_{\text{ref}}$, then $T_0 = 1$

The set of non-dimensionalized governing equations was obtained as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0 \quad (6)$$

$$\frac{\partial (\rho \vec{V})}{\partial t} + \nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla p + \frac{M_{\text{ref}}}{\text{Re}_{\text{ref}}} \nabla \cdot \vec{\tau} \quad (7)$$

$$\frac{\partial}{\partial t} \rho E + \nabla \cdot [\vec{V}(\rho E + p)] = \frac{M_{\text{ref}}}{\text{Re}_{\text{ref}}} \nabla \cdot (\kappa \nabla T) + \frac{M_{\text{ref}}}{\text{Re}_{\text{ref}}} \nabla \cdot (\vec{\tau} \cdot \vec{V}) + \dot{Q} \quad (8)$$


where the non-dimensional κ is defined as $\kappa = \left(\frac{\mu}{\text{Pr}(\gamma - 1)} \right) \left(\frac{\gamma R}{\gamma_{\text{ref}}} \right)$ (9)

For the ease in discretization of these equations for unstructured meshes, the governing equations were written in the integral form as:

$$\frac{\partial}{\partial t} \int_V \vec{Q} dV + \int_S \vec{F}^i \cdot \vec{n} dS = \int_S \vec{F}^v \cdot \vec{n} dS \quad (10)$$

where

$$\vec{Q} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} \quad (11)$$

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$$F^i \cdot \vec{n} = \begin{bmatrix} \rho\beta \\ \rho u\beta + pn_x \\ \rho v\beta + pn_y \\ \rho w\beta + pn_z \\ \beta(\rho E + p) + pn_t \end{bmatrix} \quad (12)$$

$$\vec{F}^v \cdot \vec{n} = \left(\frac{M_{\text{ref}}}{\text{Re}_{\text{ref}}} \right) \begin{bmatrix} f_1^v \\ f_2^v \\ f_3^v \\ f_4^v \\ f_5^v \end{bmatrix} = \left(\frac{M_{\text{ref}}}{\text{Re}_{\text{ref}}} \right) \begin{bmatrix} 0 \\ \left(\tau_{xx}n_x + \tau_{yx}n_y + \tau_{zx}n_z \right) \\ \left(\tau_{xy}n_x + \tau_{yy}n_y + \tau_{zy}n_z \right) \\ \left(\tau_{xz}n_x + \tau_{yz}n_y + \tau_{zz}n_z \right) \\ u f_2^v + v f_3^v + w f_4^v + \kappa \left(n_x \frac{\partial T}{\partial x} + n_y \frac{\partial T}{\partial y} + n_z \frac{\partial T}{\partial z} \right) \end{bmatrix} \quad (13)$$

where β is the contravariant velocity component of the fluid particle with respect to the grid and is defined as:

$$\beta = un_x + vn_y + wn_z - n_t$$

The thermal equation of state for perfect a gas is:


$$T = \frac{\gamma_{\text{ref}} P}{\rho R} \quad (14)$$

Relations between enthalpy per mole, specific heat per mole at constant pressure, and temperature are:

$$\begin{aligned} \hat{C}_p^o / R_u &= a_1 \hat{T}^{-2} + a_2 \hat{T}^{-1} + a_3 + a_4 \hat{T} + a_5 \hat{T}^2 + a_6 \hat{T}^3 + a_7 \hat{T}^4 \\ \hat{h}^o / R_u &= -a_1 \hat{T}^{-1} + a_2 \ln \hat{T} + a_3 \hat{T} + \frac{1}{2} a_4 \hat{T}^2 + \frac{1}{3} a_5 \hat{T}^3 + \frac{1}{4} a_6 \hat{T}^4 + \frac{1}{5} a_7 \hat{T}^5 + a_8 \end{aligned} \quad (15)$$

Species Continuity Equations

One of the prerequisites for the chemically-reacting flow modeling is the capability to solve species transport equations. This is a result of chemical reactions, where species mass fractions can be changed and transported through convection and diffusion processes. The local mass fraction of different species with the temperature and pressure govern the local reaction. The change of species mass fractions alters the mixture temperature and density at a given pressure and enthalpy. Therefore, an accurate modeling of the species transport equation is an important step. Appropriate equations of state (i.e., thermal and caloric) need to be employed to account for the real-gas effect involving multiple species.

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The species transport equation can be written as:

$$\frac{\partial \rho \alpha_i}{\partial t} + \nabla \cdot (\rho \alpha_i \vec{V}) - \nabla \cdot (D_i \nabla \rho \alpha_i) = \dot{\omega}_i \quad (16)$$

where ρ and \vec{V} are the mean density and velocity vector, D_i , α_i , and $\dot{\omega}_i$ are diffusion coefficient, species mass fraction, and source term of i -th species, respectively.

Using an eddy viscosity model, the diffusion coefficient can be written as:

$$D_i = \frac{\mu_t}{S_{c,t}} \nabla \alpha_i \quad (17)$$

Therefore, the species transport equation can be written as:


$$\frac{\partial \rho \alpha_i}{\partial t} + \nabla \cdot (\rho \vec{V} \alpha_i) = \frac{M}{\text{Re}_{\text{ref}}} \nabla \cdot \left(\left(\frac{\mu}{S_c} + \frac{\mu_t}{S_{c,t}} \right) \nabla \alpha_i \right) + \dot{\omega}_i \quad (18)$$

Integrating over the control volume and applying the divergence theorem, Equation 18 reduces to:

$$\int_{\Omega} \frac{\partial \rho \alpha_i}{\partial t} dV + \int_{\partial \Omega} \rho \alpha_i \vec{V} \cdot \vec{n} dA = \frac{M}{\text{Re}_{\text{ref}}} \int_{\partial \Omega} \left(\frac{\mu}{S_c} + \frac{\mu_t}{S_{c,t}} \right) \nabla \alpha_i \cdot \vec{n} dA + \int_{\Omega} \dot{\omega}_i dV \quad (19)$$

where $i = 1, 2, \dots, NS$ and NS is the number of species

For modeling chemical reactions, the species source term can be evaluated based on local species mass fractions and thermal state using either equilibrium or finite-rate chemistry. The species transport equation can be solved either independently (i.e., segregated approach) or by coupling with other governing equations (i.e., coupled approach). For the segregated approach, the species equation can be solved with the same time-step size as other governing equations, or with a smaller time-step size than other equations due to the disparate time-scale between flow and chemical reactions. The segregated approach requires sub-iterations to ensure convergence. The coupled approach does not need sub-iterations, but is limited to use the same time-step size for all equations, and thus requires large computer memory to store the Jacobian matrix, especially when there are a large number of species involved.

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For the source term of the species transport equation, it can be solved using an explicit or implicit approach. Each of these methods has advantages and disadvantages. In the case of explicit methods, the source term will be treated explicitly so that it is computationally efficient. However, the stability and accuracy are sacrificed due to the stiffness of the source term. In the case of implicit schemes, the sources terms will be coupled together and treated implicitly. This increases the slow solver stability, but the computational efficiency will be compromised because of the need for the solution of the denser matrix system.

Equilibrium Chemistry Model

The general form of chemical reactions can be expressed as:

$$\sum_{i=1}^{NS} \nu'_{ji} \Phi_i \xrightleftharpoons[K_{b,j}]{K_{f,j}} \sum_{i=1}^{NS} \nu''_{ji} \Phi_i \quad (20)$$

where ν'_{ji} and ν''_{ji} are the stoichiometric coefficients of species “ i ” in forward and backward reactions “ j ”, $K_{f,j}$ and $K_{b,j}$ are the forward and backward reaction rates of the j^{th} reaction, Φ_i is the name of i -th species, and NS is the total number of species.


The equilibrium chemistry model assumes that the forward and backward reactions are in the equilibrium state. In this case, the species mass fractions are determined based on the local thermal state (i.e., pressure and mixture energy) and element balance (i.e., chemical elements cannot be created or destroyed). Based on these principles, a Gibbs energy minimization method can be devised to evaluate the equilibrium species mass fraction (α_i^{n+1}). There are two ways to model the equilibrium chemistry with species transport. The first approach is to assume that reaction takes place instantly (i.e., infinitesimal time), where the species transport equation is solved with zero source term. After the species equation is solved, the equilibrium chemistry is used to determine the new species mass fraction based on the local mass fractions and thermal state. The second approach is to treat the convection, diffusion, and reaction processes that occur simultaneously, and evaluate the source term as:

$$\dot{\omega}_i = \frac{\rho(\alpha_i^{n+1} - \alpha_i^n)}{\Delta t} \quad (21)$$

The chemical equilibrium constant can be used to calculate the reverse rate constant if the forward rate constant is known.

Limitations of the equilibrium chemistry include:

1. Equilibrium chemistry assumption is valid only at high temperature and high pressure when the reaction is extremely fast,

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2. Fuel combustion (e.g., heavy hydrocarbon fuel) does not follow the equilibrium chemistry, especially at the fuel-rich condition,
3. The occurrence of soot and/or nitrogen oxide is controlled by the kinetic chemistry, and is not in chemical equilibrium,
4. Ignition and flame extinctions are not equilibrium processes, and are dependent on kinetic rates, and
5. The equilibrium chemistry cannot be used to determine the flame front location.

Finite-rate Chemistry Model

For a finite-rate chemistry model, which assumes all chemical reactions occur at a finite rate, the source term in Equation 19 is calculated based on the reaction processes, their associated kinetic rates, local species mass fractions, pressure, temperature, and the presence of a catalyst or inhibitor. The source term due to chemical reaction can be expressed as:

$$\dot{\omega}_i = M_i \sum_{j=1}^{NR} \nu_{ji} \left\{ K_{f,j} \prod_{l=1}^{NS} \left(\frac{\rho \alpha_l}{M_l} \right)^{r_{jl}} - K_{b,j} \prod_{l=1}^{NS} \left(\frac{\rho \alpha_l}{M_l} \right)^{r_{jl}^*} \right\} \quad (22)$$


where M_i is the molecular weight of species i , and NR is the total number of reactions. The chemical reaction rates in Equation 22 controls the rate of species formation and destruction. For example, higher temperature and pressure will result in a faster reaction rate. The reaction rate formulated in the empirical Arrhenius form is:

$$K_f = AT^B \exp[-E_a/R_u T] \quad (23)$$

where A , B , E_a are empirical constants. As described earlier, there are two ways of calculating the species source term. For the explicit method, since it is numerically unstable and inaccurate, some researchers employed the penalty function method to minimize the numerical error and improve the numerical stability.

In the method, the time-step size of the species equation is determined by:

$$\frac{1}{\Delta t} = \max_i \left\{ \frac{\dot{\omega}_i}{\rho(\Delta\alpha_i)_a} \right\} \quad (24)$$

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where $(\Delta\alpha)_a$ is the specified allowable maximum species mass fraction change. However, for a stiff reaction model, the calculated time-step size can become small, and thus requires a large number of sub-iterations. For the implicit method, since all the species involved in the source term are coupled and treated implicitly, the Taylor series expansion is employed to linearize the source term. Because the solution of a matrix is involved in the implicit scheme, it is less computationally efficient, but is more stable and accurate.

Linearization of the Inviscid Flux

Representing the conserved variable vector Q as:

$$\vec{Q} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \\ Q_5 \end{bmatrix} \quad (25)$$


The contravariant velocity can be represented as:

$$\theta = \frac{1}{Q_1} (Q_2 n_x + Q_3 n_y + Q_4 n_z) \quad (26)$$

Using Equation 26, the inviscid flux vector can be written as:

$$\vec{F}^i \cdot \vec{n} = \begin{bmatrix} f_1^i \\ f_2^i \\ f_3^i \\ f_4^i \\ f_5^i \end{bmatrix} = \begin{bmatrix} -n_t Q_1 + n_x Q_2 + n_y Q_3 + n_z Q_4 \\ \frac{Q_2}{Q_1} (-n_t Q_1 + n_x Q_2 + n_y Q_3 + n_z Q_4) + n_x p \\ \frac{Q_3}{Q_1} (-n_t Q_1 + n_x Q_2 + n_y Q_3 + n_z Q_4) + n_y p \\ \frac{Q_4}{Q_1} (-n_t Q_1 + n_x Q_2 + n_y Q_3 + n_z Q_4) + n_z p \\ \frac{Q_5}{Q_1} (-n_t Q_1 + n_x Q_2 + n_y Q_3 + n_z Q_4) + \frac{p}{Q_1} (n_x Q_2 + n_y Q_3 + n_z Q_4) \end{bmatrix} \quad (27)$$

Equation 27 can be differentiated with respect to Equation 25 to get the inviscid flux Jacobian.

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Each component of the inviscid flux vector can be represented as $A_{jk} = \frac{\partial f_j^i}{\partial Q_k}$, which will result in:

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{bmatrix} \quad (28)$$

For the linearization of the flux vector, it is assumed that the ratio of specific heats is locally constant. Based on this assumption, each term in Equation 28 can be expressed as:

$$A = \begin{bmatrix} -n_t & n_x & n_y & n_z & 0 \\ n_x \phi - u\theta & n_x(2-\gamma)u + U & n_y u - n_x(\gamma-1)v & n_z u - n_x(\gamma-1)w & n_x(\gamma-1) \\ n_y \phi - v\theta & n_x v - n_y(\gamma-1)u & n_y(2-\gamma)v + U & n_z v - n_y(\gamma-1)w & n_y(\gamma-1) \\ n_z \phi - w\theta & n_x w - n_z(\gamma-1)u & n_y w - n_z(\gamma-1)v & n_z(2-\gamma)w + U & n_z(\gamma-1) \\ \left(2\phi - \frac{\gamma E}{\rho}\right)\theta & n_x \left(\frac{\gamma E}{\rho} - \phi\right) - (\gamma-1)u\theta & n_y \left(\frac{\gamma E}{\rho} - \phi\right) - (\gamma-1)v\theta & n_z \left(\frac{\gamma E}{\rho} - \phi\right) - (\gamma-1)w\theta & \gamma\theta - n_t \end{bmatrix} \quad (29)$$


where

$$\theta = un_x + vn_y + wn_z \quad (30)$$

$$\phi = \frac{\gamma-1}{2}(u^2 + v^2 + w^2) \quad (31)$$

Linearization of Viscous Terms

The viscous terms involves the gradients of the primitive variables. Therefore, linearization of the viscous terms will be simpler if primitive variables are used as the independent variable. To linearize the viscous flux with respect to the conserved variables, the Jacobian, based on the primitive variables, can be multiplied by the linearization of the primitive variables with respect to the conserved variables.

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The variable vector q selected for this linearization procedure is taken as:

$$\bar{q} = \begin{bmatrix} \rho \\ u \\ v \\ w \\ p \end{bmatrix} = \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2/Q_1 \\ Q_3/Q_1 \\ Q_4/Q_1 \\ q_5 \end{bmatrix} \quad (32)$$


Hence, Jacobian resulting from the linearization of the primitive variable with respect to the conserved variable can be written as:

$$\frac{\partial \bar{q}}{\partial \bar{Q}} = \begin{bmatrix} \frac{\partial q_1}{\partial Q_1} & \frac{\partial q_1}{\partial Q_2} & \frac{\partial q_1}{\partial Q_3} & \frac{\partial q_1}{\partial Q_4} & \frac{\partial q_1}{\partial Q_5} \\ \frac{\partial q_2}{\partial Q_1} & \frac{\partial q_2}{\partial Q_2} & \frac{\partial q_2}{\partial Q_3} & \frac{\partial q_2}{\partial Q_4} & \frac{\partial q_2}{\partial Q_5} \\ \frac{\partial q_3}{\partial Q_1} & \frac{\partial q_3}{\partial Q_2} & \frac{\partial q_3}{\partial Q_3} & \frac{\partial q_3}{\partial Q_4} & \frac{\partial q_3}{\partial Q_5} \\ \frac{\partial q_4}{\partial Q_1} & \frac{\partial q_4}{\partial Q_2} & \frac{\partial q_4}{\partial Q_3} & \frac{\partial q_4}{\partial Q_4} & \frac{\partial q_4}{\partial Q_5} \\ \frac{\partial q_5}{\partial Q_1} & \frac{\partial q_5}{\partial Q_2} & \frac{\partial q_5}{\partial Q_3} & \frac{\partial q_5}{\partial Q_4} & \frac{\partial q_5}{\partial Q_5} \end{bmatrix} \quad (33)$$

Using the relation between primitive and conserve variable, the above Jacobian can be reduced to:

$$\frac{\partial \bar{q}}{\partial \bar{Q}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -u/\rho & 1/\rho & 0 & 0 & 0 \\ -v/\rho & 0 & 1/\rho & 0 & 0 \\ -w/\rho & 0 & 0 & 1/\rho & 0 \\ \frac{\partial p}{\partial \rho} & -(\gamma-1)u & -(\gamma-1)v & -(\gamma-1)w & \gamma-1 \end{bmatrix} \quad (34)$$

The details of this derivation are provided in Appendix A. The linearization of pressure for real-gas is provided in Appendix B.

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From Equation 14, Equation 35 can be obtained as:

$$dT = -\frac{T}{\rho} d\rho + \frac{\gamma_{\text{ref}}}{\rho R} dp \quad (35)$$

Hence,


$$\frac{\partial T}{\partial \vec{q}} = \begin{bmatrix} -\frac{T}{\rho} & 0 & 0 & 0 & \frac{\gamma_{\text{ref}}}{\rho R} \end{bmatrix} \quad (36)$$

Combining Equations 34 and 36 produces:

$$\begin{aligned} \frac{\partial T}{\partial \vec{Q}} &= \begin{bmatrix} \frac{\partial T}{\partial Q_1} & \frac{\partial T}{\partial Q_2} & \frac{\partial T}{\partial Q_3} & \frac{\partial T}{\partial Q_4} & \frac{\partial T}{\partial Q_5} \end{bmatrix} = \frac{\partial T}{\partial \vec{q}} \frac{\partial \vec{q}}{\partial \vec{Q}} \\ &= \begin{bmatrix} -\frac{T}{\rho} & 0 & 0 & 0 & \frac{\gamma_{\text{ref}}}{\rho R} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -u/\rho & 1/\rho & 0 & 0 & 0 \\ -v/\rho & 0 & 1/\rho & 0 & 0 \\ -w/\rho & 0 & 0 & 1/\rho & 0 \\ \frac{\partial p}{\partial \rho} & -(\gamma-1)u & -(\gamma-1)v & -(\gamma-1)w & \gamma-1 \end{bmatrix} \\ &= \begin{bmatrix} -\frac{T}{\rho} + \frac{\gamma_{\text{ref}}}{\rho R} \frac{\partial p}{\partial \rho} & \frac{-\gamma_{\text{ref}}(\gamma-1)u}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)v}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)w}{\rho R} & \frac{\gamma_{\text{ref}}(\gamma-1)}{\rho R} \end{bmatrix} \\ &= \begin{bmatrix} -\frac{T}{\rho} + \frac{\gamma_{\text{ref}}(\gamma-1)V^2}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)u}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)v}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)w}{\rho R} & \frac{\gamma_{\text{ref}}(\gamma-1)}{\rho R} \end{bmatrix} \end{aligned} \quad (37)$$

The spatial derivatives any primitive variable ϕ at the interface between two adjacent cells can be calculated as:

$$\begin{aligned} \phi_x &= \frac{\partial \phi}{\partial x} = \Gamma_x \Delta \phi; \quad \Gamma_x = \frac{n_x}{n_x \Delta x + n_y \Delta y + n_z \Delta z} \\ \phi_y &= \frac{\partial \phi}{\partial y} = \Gamma_y \Delta \phi; \quad \Gamma_y = \frac{n_y}{n_x \Delta x + n_y \Delta y + n_z \Delta z} \\ \phi_z &= \frac{\partial \phi}{\partial z} = \Gamma_z \Delta \phi; \quad \Gamma_z = \frac{n_z}{n_x \Delta x + n_y \Delta y + n_z \Delta z} \end{aligned} \quad (38)$$

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and $\Delta\phi = \phi_R - \phi_L$ where ϕ_R and ϕ_L are the values of ϕ at the center of right and left cells, as shown in Figure 7.1-1.

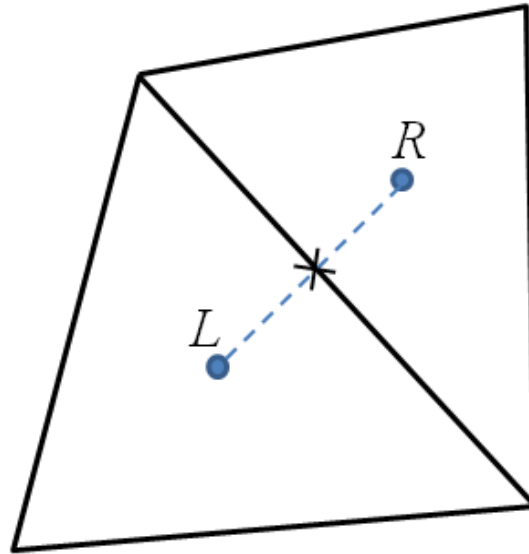



Figure 7.1-1. Nomenclature of a Face and it's Neighbors

Hence, the spatial derivatives of a dependent variable at the cell face can be linearized by the conservative \vec{Q} as:

$$\frac{\partial \phi_x}{\partial \vec{Q}} = \Gamma_x \frac{\partial(\Delta\phi)}{\partial \vec{Q}} = \Gamma_x \left(\frac{\partial(\phi_R - \phi_L)}{\partial \vec{Q}} \right) \quad (39)$$

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Therefore,

$$\frac{\partial \phi_x}{\partial \bar{Q}_R} = \Gamma_x \left(\frac{\partial \phi_R}{\partial \bar{Q}_R} \right) \quad (40)$$

$$\frac{\partial \phi_x}{\partial \bar{Q}_L} = -\Gamma_x \left(\frac{\partial \phi_L}{\partial \bar{Q}_L} \right) \quad (41)$$

Equation 13 can be differentiated with respect to Equation 25 to get the viscous flux Jacobian.

Each component of the viscous flux vector can be represented as $B_{jk} = \frac{\partial f_j^v}{\partial Q_k}$ and this will result

in:

$$B = \begin{bmatrix} B_{11} & B_{12} & B_{13} & B_{14} & B_{15} \\ B_{21} & B_{22} & B_{23} & B_{24} & B_{25} \\ B_{31} & B_{32} & B_{33} & B_{34} & B_{35} \\ B_{41} & B_{42} & B_{43} & B_{44} & B_{45} \\ B_{51} & B_{52} & B_{53} & B_{54} & B_{55} \end{bmatrix} \quad (42)$$

By substituting Equations 34, 37, and 39, each components of the viscous flux Jacobian can be expressed as:


$$B_{11} = B_{12} = B_{13} = B_{14} = B_{15} = 0 \quad (43)$$

$$B_{2j} = \frac{\partial f_2^v}{\partial (Q_c)_j} = \left(n_x \frac{\partial \tau_{xx}}{\partial (Q_c)_j} + n_y \frac{\partial \tau_{yx}}{\partial (Q_c)_j} + n_z \frac{\partial \tau_{zx}}{\partial (Q_c)_j} \right) \quad (44)$$

$$B_{3j} = \frac{\partial f_3^v}{\partial (Q_c)_j} = \left(n_x \frac{\partial \tau_{xy}}{\partial (Q_c)_j} + n_y \frac{\partial \tau_{yy}}{\partial (Q_c)_j} + n_z \frac{\partial \tau_{zy}}{\partial (Q_c)_j} \right) \quad (45)$$

$$B_{4j} = \frac{\partial f_4^v}{\partial (Q_c)_j} = \left(n_x \frac{\partial \tau_{xz}}{\partial (Q_c)_j} + n_y \frac{\partial \tau_{yz}}{\partial (Q_c)_j} + n_z \frac{\partial \tau_{zz}}{\partial (Q_c)_j} \right) \quad (46)$$

$$\begin{aligned} B_{5j} &= \frac{\partial f_5^v}{\partial (Q_c)_j} = \frac{\partial (u_f f_2^v)}{\partial (Q_c)_j} + \frac{\partial (v_f f_3^v)}{\partial (Q_c)_j} + \frac{\partial (w_f f_4^v)}{\partial (Q_c)_j} + \kappa \left(n_x \frac{\partial T_x}{\partial (Q_c)_j} + n_y \frac{\partial T_y}{\partial (Q_c)_j} + n_z \frac{\partial T_z}{\partial (Q_c)_j} \right) \\ &= u_f B_{2j} + v_f B_{3j} + w_f B_{4j} + \kappa \left(n_x \frac{\partial T_x}{\partial (Q_c)_j} + n_y \frac{\partial T_y}{\partial (Q_c)_j} + n_z \frac{\partial T_z}{\partial (Q_c)_j} \right) \end{aligned} \quad (47)$$

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where C represents either cell on the left or the cell on the right-side of the face and j represents the column number.

7.2 Numerical Implementation

An overall flow diagram of the USM3D code main time loop with the current modifications to add real-gas capability is given below. The sections highlighted in bold letters represent new code additions. The USM3D code was modified to add variable ratio of specific heats. The modifications added to the different code modules are described in this section.

DO 25 nts UN = 1, ntstep

Move grid

Qnode

UBC2

DO 10 nts = 1, niter

UCTime

Limiter

Turbulence model -> Update viscosity

Calculate species source terms based on equilibrium or finite chemistry

Solve species transport equations

Save $(\rho\alpha)^{n+1}$

Viscous flux

Update (Implicit scheme)

Calculate RHS


Calculate LHS

Calculate ΔQ

Update state variables

Update species mass fraction $\alpha^{n+1} = \frac{(\rho\alpha)^{n+1}}{\rho^{n+1}}$

Calculate new species mass fraction based on equilibrium chemistry model if the effect is not included in the species source term

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Update temperature and pressure using new species mass fractions and state variables

Q_{node}

UBC2

Force

.....

10 Continue

25 Continue

Roe's Approximate Riemann Solver

Based on Roe's approximate Riemann solver, the numerical flux that crosses a cell-face can be written as:

$$F_{LR} = \frac{1}{2} \left(F(Q_L) + F(Q_R) - |\bar{A}| (Q_R - Q_L) \right) \quad (48)$$

where L and R represent the cells on the left and right sides of the face respectively, Q is the conserved variable vector, and $|\bar{A}|$ is the Roe averaged matrix. The flux vector $F(Q)$ is defined as:


$$F(Q) = \begin{bmatrix} \rho U \\ \rho u U + p n_x \\ \rho v U + p n_y \\ \rho w U + p n_z \\ U(\rho E + p) \end{bmatrix} \quad (49)$$

where E is the total energy per unit mass and U is the contravariant velocity. The variables used in the Roe averaged matrix are evaluated as:

$$\bar{\rho} = \sqrt{\rho_L \rho_R} \quad (50)$$

$$\bar{u} = \frac{(u_L + u_R \sqrt{\rho_R / \rho_L})}{1 + \sqrt{\rho_R / \rho_L}} \quad (51)$$

$$\bar{v} = \frac{(v_L + v_R \sqrt{\rho_R / \rho_L})}{1 + \sqrt{\rho_R / \rho_L}} \quad (52)$$

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$$\bar{w} = \frac{(w_L + w_R \sqrt{\rho_R / \rho_L})}{1 + \sqrt{\rho_R / \rho_L}} \quad (53)$$

$$\bar{h}_0 = \frac{(h_{0L} + h_{0R} \sqrt{\rho_R / \rho_L})}{1 + \sqrt{\rho_R / \rho_L}} \quad (54)$$

The diffusion term (i.e., last term in Equation 48) can be split it into three components as:

$$|\bar{A}|(Q_R - Q_L) = |\Delta\bar{F}_1| + |\Delta\bar{F}_2| + |\Delta\bar{F}_3| \quad (55)$$

$$\text{where, } |\Delta\bar{F}_1| = |\bar{U}| \left\{ \left(\Delta\rho - \frac{\Delta p}{\bar{a}^2} \right) \begin{bmatrix} 1 \\ \bar{u} \\ \bar{v} \\ \bar{w} \\ \frac{1}{2}(\bar{u}^2 + \bar{v}^2 + \bar{w}^2) \end{bmatrix} + \bar{\rho} \begin{bmatrix} 0 \\ \Delta u - n_x \Delta U \\ \Delta v - n_y \Delta U \\ \Delta w - n_z \Delta U \\ \bar{u} \Delta u + \bar{v} \Delta v + \bar{w} \Delta w - \bar{U} \Delta U \end{bmatrix} \right\} \quad (56)$$

$$|\Delta\bar{F}_{4,5}| = |\bar{U} \pm \bar{a}| \begin{bmatrix} 1 \\ \bar{u} \pm n_x \bar{a} \\ \bar{v} \pm n_y \bar{a} \\ \bar{w} \pm n_z \bar{a} \\ \bar{h}_0 \pm \bar{U} \bar{a} \end{bmatrix} \left(\frac{\Delta p \pm \bar{\rho} \bar{a} \Delta U}{2\bar{a}^2} \right) \quad (57)$$

where Δ represents the change in the variable value between the cell on the right and cell on the left.

The different components (i.e., mass, momentum, and energy) of the flux vector can be written:

$$f_1 = \frac{(\rho U)_L + (\rho U)_R}{2} - \frac{|\bar{U}|}{2} \left(\Delta\rho - \frac{\Delta p}{\bar{a}^2} \right) - |\bar{U} + \bar{a}| \left(\frac{\Delta p + \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) - |\bar{U} - \bar{a}| \left(\frac{\Delta p - \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) \quad (58)$$



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$$f_2 = \frac{(\rho u U)_L + (\rho u U)_R + (p_L + p_R)n_x}{2} - \frac{|\bar{U}|}{2} \left[\bar{u} \left(\Delta \rho - \frac{\Delta p}{\bar{a}^2} \right) + \bar{\rho} (\Delta u - n_x \Delta U) \right] - |\bar{U} + \bar{a}| \left(\frac{\Delta p + \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) (\bar{u} + n_x \bar{a}) - |\bar{U} - \bar{a}| \left(\frac{\Delta p - \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) (\bar{u} - n_x \bar{a}) \quad (59)$$


$$f_3 = \frac{(\rho v U)_L + (\rho v U)_R + (p_L + p_R)n_y}{2} - \frac{|\bar{U}|}{2} \left[\bar{v} \left(\Delta \rho - \frac{\Delta p}{\bar{a}^2} \right) + \bar{\rho} (\Delta v - n_y \Delta U) \right] - |\bar{U} + \bar{a}| \left(\frac{\Delta p + \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) (\bar{v} + n_y \bar{a}) - |\bar{U} - \bar{a}| \left(\frac{\Delta p - \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) (\bar{v} - n_y \bar{a}) \quad (60)$$

$$f_4 = \frac{(\rho w U)_L - (\rho w U)_R + (p_L + p_R)n_z}{2} - \frac{|\bar{U}|}{2} \left[\bar{w} \left(\Delta \rho - \frac{\Delta p}{\bar{a}^2} \right) + \bar{\rho} (\Delta w - n_z \Delta U) \right] - |\bar{U} + \bar{a}| \left(\frac{\Delta p + \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) (\bar{w} + n_z \bar{a}) - |\bar{U} - \bar{a}| \left(\frac{\Delta p - \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) (\bar{w} - n_z \bar{a}) \quad (61)$$

$$f_5 = \frac{1}{2} \left[\begin{aligned} & (\rho U(E + p))_L + (\rho U(E + p))_R - \\ & \left[\bar{U} \left(\left(\Delta \rho - \frac{\Delta p}{\bar{a}^2} \right) \frac{1}{2} (\bar{u}^2 + \bar{v}^2 + \bar{w}^2) \right) - \bar{\rho} (\bar{u} \Delta u + \bar{v} \Delta v + \bar{w} \Delta w - \bar{U} \Delta U) \right] - \\ & \left[|\bar{U} + \bar{a}| \left(\frac{\Delta p + \bar{\rho} \bar{a} \Delta U}{2\bar{a}^2} \right) (\bar{h}_0 + \bar{U} \bar{a}) - |\bar{U} - \bar{a}| \left(\frac{\Delta p - \bar{\rho} \bar{a} \Delta U}{2\bar{a}^2} \right) (\bar{h}_0 + \bar{U} \bar{a}) \right] \end{aligned} \right] \quad (62)$$

$$f_5 = \frac{(\rho U h_0)_L + (\rho U h_0)_R}{2} - \frac{|\bar{U}|}{2} \left(\Delta \rho - \frac{\Delta p}{\bar{a}^2} \right) \frac{\bar{V}^2}{2} - \frac{|\bar{U}|}{2} \bar{\rho} (\bar{u} \Delta u + \bar{v} \Delta v + \bar{w} \Delta w - \bar{U} \Delta U) - |\bar{U} + \bar{a}| \left(\frac{\Delta p + \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) (\bar{h}_0 + \bar{U} \bar{a}) - |\bar{U} - \bar{a}| \left(\frac{\Delta p - \bar{\rho} \bar{a} \Delta U}{4\bar{a}^2} \right) (\bar{h}_0 - \bar{U} \bar{a}) \quad (63)$$

For flows with multiple species, the ratio of specific heats used in the Roe averaged matrix is evaluated in different ways by different authors. Two of the commonly used methods are described in the following sections.

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Methods used by Luke [ref. 2]

The ratio of specific heats is evaluated as:

$$\bar{\gamma} = 1 + \frac{\bar{R}}{C_v^*} \quad (64)$$

where,

$$\bar{R} = \sum_{s=1}^{NS} \bar{\alpha}_s R_s \quad (65)$$

$$C_v^* = \sum_{s=1}^{NS} \bar{\alpha}_s C_{vs}^*, \text{ and} \quad (66)$$

$$C_{vs}^* = \frac{1}{T_R - T_L} \int_{T_L}^{T_R} C_{vs} dT \quad (67)$$

$$\bar{\alpha}_s = \frac{(\alpha_{s,L} + \alpha_{s,R} \sqrt{\rho_R / \rho_L})}{1 + \sqrt{\rho_R / \rho_L}} \quad (68)$$

$$\bar{T} = \frac{(T_L + T_R \sqrt{\rho_R / \rho_L})}{1 + \sqrt{\rho_R / \rho_L}} \quad (69)$$

$$\bar{e}_s = \frac{(e_{s,L} + e_{s,R} \sqrt{\rho_R / \rho_L})}{1 + \sqrt{\rho_R / \rho_L}} \quad (70)$$

The speed of sound is calculated as:


$$\bar{a}^2 = (\bar{\gamma} - 1) \left(\bar{h}_0 - \frac{1}{2} (\bar{u}^2 + \bar{v}^2 + \bar{w}^2) + C_v^* \bar{T} - \sum_{s=1}^{NS} \bar{\alpha}_s \bar{e}_s \right) \quad (71)$$

Method used by Molvik and Merkle [ref. 3]

Molvik and Merkle used the following approach to calculate the speed of sound and the ratio of specific heats. The initial estimation for the speed of sound, ratio of specific heats, and the chemical source term are defined as:

$$a = \frac{a_L + a_R}{2} \quad (72)$$

$$\gamma = \frac{\gamma_L + \gamma_R}{2} \quad (73)$$

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$$D_s = \frac{D_{sL} + D_{sR}}{2} \quad (74)$$

These values are refined to meet Roe's criteria as:

$$\bar{D}_s = \frac{D_s - \bar{a}^4 \Delta \rho_s \delta p / \chi}{1 - \Delta p \delta p / \chi} \quad (75)$$

$$\bar{\gamma} = \frac{\gamma - 1}{1 - \Delta p \delta p / \chi} + 1 \quad (76)$$

where Δ represents the change in the value between right and left states, and the other variables appearing in Equation 76 are calculated as:

$$\delta p = \Delta p + \sum_{s=1}^{NS} D_s \Delta \rho_s - (\gamma - 1)(\Delta(\rho h) - \Delta p) \quad (77)$$

$$\chi = \sum_{s=1}^{NS} (a^2 \Delta \rho_s)^2 + (\Delta p)^2 \quad (78)$$

The Roe averaged speed of sound (\bar{a}) of sound is calculated as:

$$\bar{a}^2 = (\bar{\gamma} - 1)\bar{h} - \sum_{s=1}^{NS} \bar{\rho}_s \bar{D}_s \quad (79)$$

Methodology Implemented in USM3D Code


Currently, in the USM3D code, the Roe averaged speed of sound is calculated based on constant specific heat assumption expressed as:

$$\bar{a}^2 = \gamma \bar{R} \bar{T} = \gamma(\gamma - 1) \bar{C}_v \bar{T} = \gamma(\gamma - 1) \bar{e} = \gamma(\gamma - 1) \left(\bar{E} - \frac{1}{2} (\bar{u}^2 + \bar{v}^2 + \bar{w}^2) \right) \quad (80)$$

This has been modified to calculate the speed of sound based on variable ratio of specific heats. The Roe averaged density, velocity components, and total energy were calculated using Equations 50 through 54. The other Roe averaged correlations used for different flow variables are listed as:

$$\bar{\alpha}_s = \frac{(\alpha_{s,L} + \alpha_{s,R} \sqrt{\rho_R / \rho_L})}{1 + \sqrt{\rho_R / \rho_L}} \quad (81)$$

$$\bar{e} = \bar{E} - \frac{1}{2} (\bar{u}^2 + \bar{v}^2 + \bar{w}^2) = \sum_{s=1}^{NS} \bar{\alpha}_s \bar{e}_s \quad (82)$$

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Since $d\bar{e} = \bar{C}_v d\bar{T}$, the Newton-Raphson method was used to solve for $\bar{T} (= \bar{T}^{n+1})$ as:

$$\bar{T}^{n+1} = \bar{T}^n + \frac{\bar{e}^{n+1} - \bar{e}^n}{\bar{C}_v^n} \quad (83)$$

$$\bar{T}^{n+1} = \bar{T}^n + \frac{\frac{\bar{e}^{n+1}}{\bar{R}} - \frac{\bar{e}^n}{\bar{R}}}{\bar{C}_v^n / \bar{R}} \quad (84)$$

$$\frac{\bar{C}_v}{\bar{R}} = \frac{\bar{C}_p - \bar{R}}{\bar{R}} = \frac{\bar{C}_p}{\bar{R}} - 1 = \frac{\bar{C}_p^o}{R_u} - 1 = \sum_{s=1}^{NS} \bar{n}_s \frac{(C_p^o)_s}{R_u} - 1 \quad (85)$$

$$\frac{\bar{e}}{\bar{R}} = \frac{\bar{h} - \bar{R}\bar{T}}{\bar{R}} = \frac{\bar{h}}{\bar{R}} - \bar{T} = \frac{\bar{h}^o}{R_u} - \bar{T} = \sum_{s=1}^{NS} \bar{n}_s \frac{\bar{h}_s^o}{R_u} - \bar{T} \quad (86)$$

$$\bar{n}_s = \frac{\bar{\alpha}_s / M_s}{\sum_{s=1}^{NS} (\bar{\alpha}_s / M_s)} \quad (87)$$

$$(\bar{C}_p^o)_s / R_u = (a_1 \bar{T}^{-2} + a_2 \bar{T}^{-1} + a_3 + a_4 \bar{T} + a_5 \bar{T}^2 + a_6 \bar{T}^3 + a_7 \bar{T}^4)_s \quad (88)$$

$$\bar{h}_s^o / R_u = (-a_1 \bar{T}^{-1} + a_2 \ln \bar{T} + a_3 \bar{T} + \frac{1}{2} a_4 \bar{T}^2 + \frac{1}{3} a_5 \bar{T}^3 + \frac{1}{4} a_6 \bar{T}^4 + \frac{1}{5} a_7 \bar{T}^5 + a_8)_s \quad (89)$$

Once the Roe-averaged temperature is obtained, \bar{a} , can be calculated based on:


$$\bar{a} = \sqrt{\bar{\gamma} \bar{R} \bar{T}} \quad (90)$$

where

$$\bar{R} = \sum_{s=1}^{NS} \bar{\alpha}_s R_s \quad (91)$$

$$R_s = \frac{R_u}{M_s} \quad (92)$$

$$\bar{\gamma} = \frac{\bar{C}_p / \bar{R}}{(\bar{C}_p / \bar{R}) - 1} \quad (93)$$

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Modifications to Boundary Conditions

Boundary Condition 0: Freestream (Supersonic Inflow)

- Specify and fix density, velocity components, species mass fraction (i.e., mixture gas constant), and pressure.
- Calculate mixture temperature and Gamma (i.e., ratio of specific heats) based on pressure, mixture density, and mixture gas constant using the thermal equation of state.
- Calculate total energy from species mass fractions and mixture temperature, and velocity based on the caloric equation of state.

Boundary Condition 1: Tangent Flow (Reflection Plane)

- Set contravariant velocity component to zero.
- Set pressure, mixture density, and species mass fractions at the boundary to be the same as the values of the cell values.
- Calculate mixture temperature and Gamma based on pressure, mixture density, and mixture gas constant using the thermal equation of state.
- Calculate total energy from species mass fractions and mixture temperature, and velocity based on the caloric equation of state.

Boundary Condition 2: Full Extrapolation (Supersonic Outflow)

- Extrapolate velocity components, pressure and mixture density at the boundary from the cell values.
- Set species mass fractions at the boundary to be the same as the values of the cell inside.
- Calculate mixture temperature and Gamma at the boundary based on pressure, mixture density, and mixture gas constant using the thermal equation of state.
- Calculate total energy at the boundary from species mass fractions and mixture temperature, and velocity based on the caloric equation of state.


Boundary Condition 3: Characteristic Inflow/Outflow (Subsonic Outer Boundaries)

Appendix C provides a detailed description.

- Assumptions
 - Species mass fractions at the boundary are the same as species mass fractions inside if the contravariant velocity is positive (i.e., outflow).
 - Species mass fractions at the boundary are the same as freestream species mass fractions if the contravariant velocity is negative (i.e., inflow).
- Use Riemann invariants to calculate the boundary contravariant velocity and the speed of sound. Use the speed of sound to calculate the temperature.

The Riemann invariants corresponding to the outgoing and incoming characteristics are given by:

$$\mathfrak{R}^+ = U + \frac{2a}{\gamma - 1}, \text{ and } \mathfrak{R}^- = U - \frac{2a}{\gamma - 1}$$

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where \mathfrak{R}^+ is corresponding to the eigenvalue, $U+a$, and \mathfrak{R}^- is corresponding to the eigenvalue $U-a$. These Riemann invariants at the boundary can be written as:

$$\mathfrak{R}_b^+ = \begin{cases} \mathfrak{R}_{\text{inside}}^+ & \text{if } U + a > 0 \\ \mathfrak{R}_{\text{freestream}}^+ & \text{if } U + a < 0 \end{cases} \quad (94)$$

$$\mathfrak{R}_b^- = \begin{cases} \mathfrak{R}_{\text{inside}}^- & \text{if } U - a > 0 \\ \mathfrak{R}_{\text{freestream}}^- & \text{if } U - a < 0 \end{cases} \quad (95)$$

The boundary contravariant velocity (U_b) and speed of sound (a_b) can be calculated by solving Equations 94 and 95. The boundary species mass fractions ($(\alpha_s)_b$) will be the same as those of the cell at the upwind side. Since:

$$a_b = \sqrt{\frac{\gamma_b R_b T_b}{\gamma_{\text{ref}}}}; \quad R_b = f(\alpha_{s,b}); \quad \text{and } \gamma_b = f(T_b, (\alpha_s)_b)$$

An iterative procedure was used to determine the boundary temperature and the ratio of specific heats based on the boundary speed of sound and species mass fractions. With the isentropic assumption between the upwind cell and the boundary, the boundary mixture density and pressure can be calculated based on the temperature (T_c) and mixture density (ρ_c) of the upwind cell as:


$$\rho_b = \left[\frac{T_b}{(T_c / \rho_c^{\gamma_b - 1})} \right]^{\frac{1}{\gamma_b - 1}}; \quad \text{and } p_b = \frac{1}{\gamma_\infty} \rho_b R_b T_b$$

Total energy at the boundary was calculated from boundary temperature, species mass fraction, and velocity components based on the caloric equation of state.

Boundary Condition 4: No-Slip (Viscous Surfaces)

Appendix D provides a detailed description.

- Stationary wall: set velocity components at the wall boundary to be zero and velocity components at the ghost point to have the opposite direction to those at the neighboring interior cell.
- Moving wall: set velocity components at the wall boundary to be the prescribed speed of the moving wall and extrapolate velocity components at the ghost point from the neighboring interior cell and wall boundary.
- Extrapolate pressure at the wall boundary from neighboring interior cells, and extrapolate pressure at the ghost point from the neighboring interior cell and wall boundary.
- Set the species mass fractions to be the same as those of the neighboring interior cells.

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- Adiabatic: in the current implementation, temperature at the wall boundary is set to the same as its neighboring interior cell.
- Isothermal: temperature at the wall boundary remains unchanged.
- Calculate mixture density: total energy at the wall boundary is calculated from temperature, pressure, species mass fraction, and velocity components based on the thermal and caloric equation of state.

Boundary Condition 5: Tangent Flow (Inviscid Aerodynamic Surface)

- Same as boundary condition 1.


Boundary Condition 44: Special no-slip (Blunt base)

- Same as boundary condition 4.
- If wall function, then it is different than boundary condition 4.

8.0 Verification of Multi-Species Capability

The implementation of the numerical models from Section 7.0 was verified using hot-gas flow conditions through a round convergent-divergent nozzle exiting into ambient air. The solutions presented in the following sections will only serve as qualitative verification of the implementation of the real-gas energy and multi-species transport equations, and are not validated against experimental data.

The configuration consists of a plenum chamber, which is represented as the small straight section on the left-side of the geometry shown in Figure 8.0-1, followed by the convergent divergent nozzle. A computational grid of 2,706,755 tetrahedral cells was constructed for one quadrant of the round nozzle configuration. Figure 8.0-1 depicts the grid clustering on one of the quadrant boundaries. The hot jet flow exits the nozzle at nominally Mach 2 into near-quiescent ambient air. The freestream Mach number is set to 0.05 for numerical purposes. The plenum is set to total pressure, p_{tot} , of 115 psi and total temperature, T_{tot} , of 2009 degR to produce a hot jet plume. The chemical composition of the plenum gas is varied to simulate different flow scenarios. The inflow boundary condition to the plenum is specified using *Engine* boundary condition in USM3D code. A description of the USM3D input parameters is presented in Appendix E.

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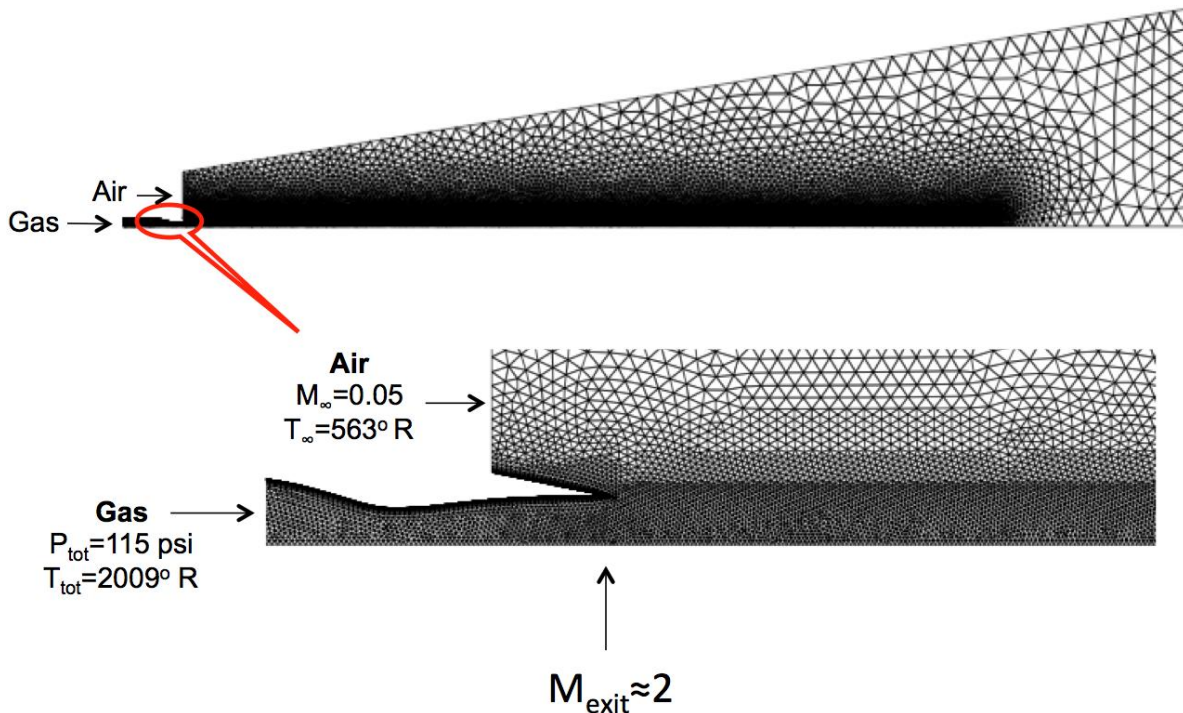


Figure 8.0-1. Triangulation on Boundary Plane of Tetrahedral Quadrant Grid for Nozzle Test Case

8.1 Comparison of Ideal and Real Gas Simulations

This section presents the comparison of the simulation results from the ideal- and real-gas versions of the USM3D code. The results confirm the expected variation of the ratio of specific heats with temperature from the modified energy equation. The multi-species transport equations are not solved in this example. In the following comparison, the real-gas is taken as air with a mixture of 73.5 percent nitrogen (N_2) and 26.5 percent oxygen (O_2). This mass fraction is assumed to be the same for the entire flowfield. In these simulations, the Courant-Friedrichs-Lewy (CFL) number is ramped from 1 to 10 in 800 iterations. The ideal-gas simulation was run for 9,000 iterations. By using 9,000 iterations for real-gas simulation, the flow was not fully developed and contour deviations for temperature and Mach number near the axis of rotation between the ideal- and real-gas simulations were noted. Therefore, the real-gas version of the USM3D code was run for 30,000 iterations. The comparison of the pressure, temperature, Mach number, and ratio of specific heats is given in Figure 8.1-1. This figure shows that contours of pressure, temperature, and Mach number are similar for both ideal- and real-air simulations. The variation of ratio of specific heats for the real-gas simulation can be seen in Figure 8.1-1(d). As expected, the ratio of specific heats is lower in the settling chamber where the temperature is high, and defuses toward the ambient gamma ratio of 1.4 as the temperature of the jet plume decreases toward the ambient condition.



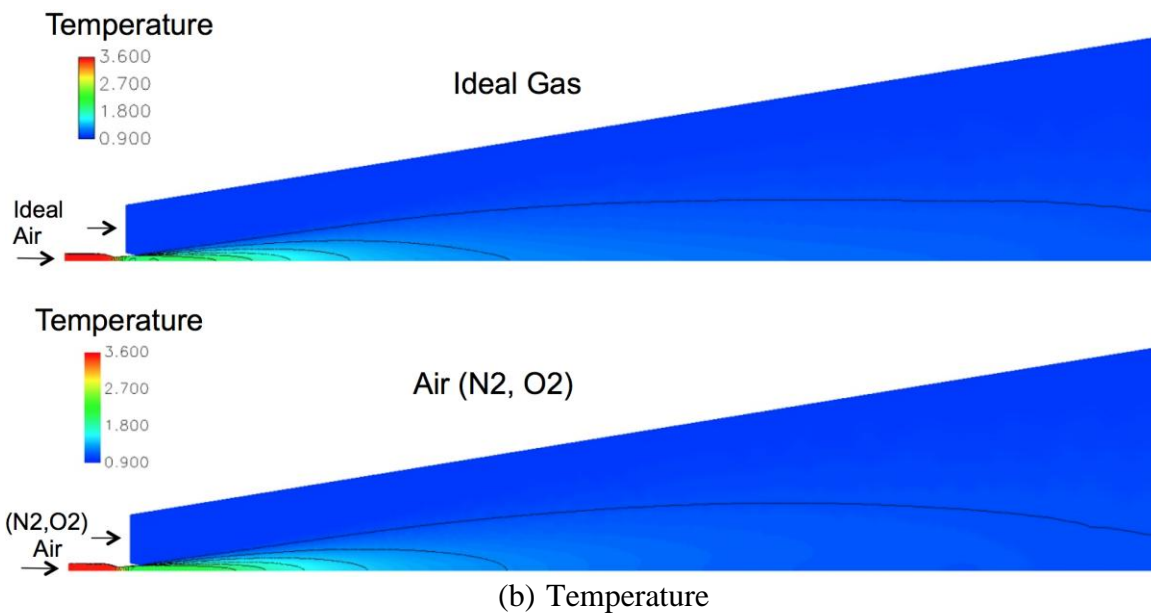
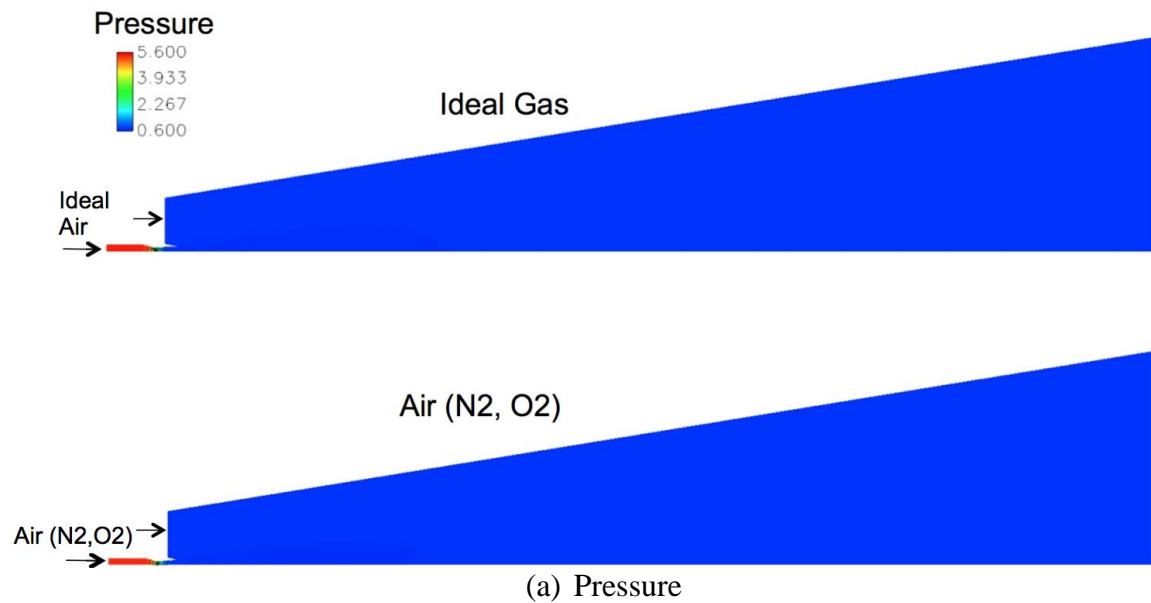
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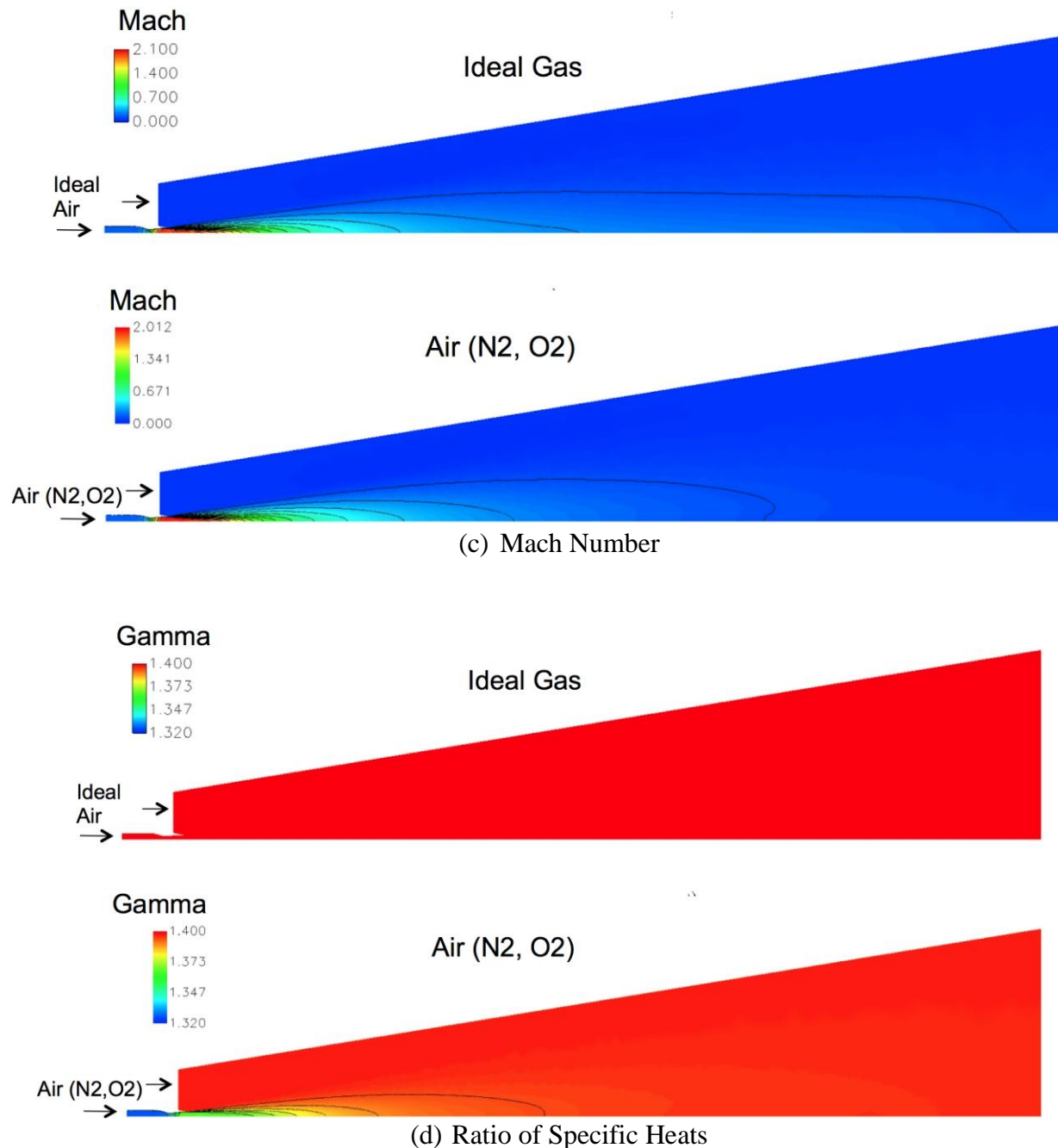

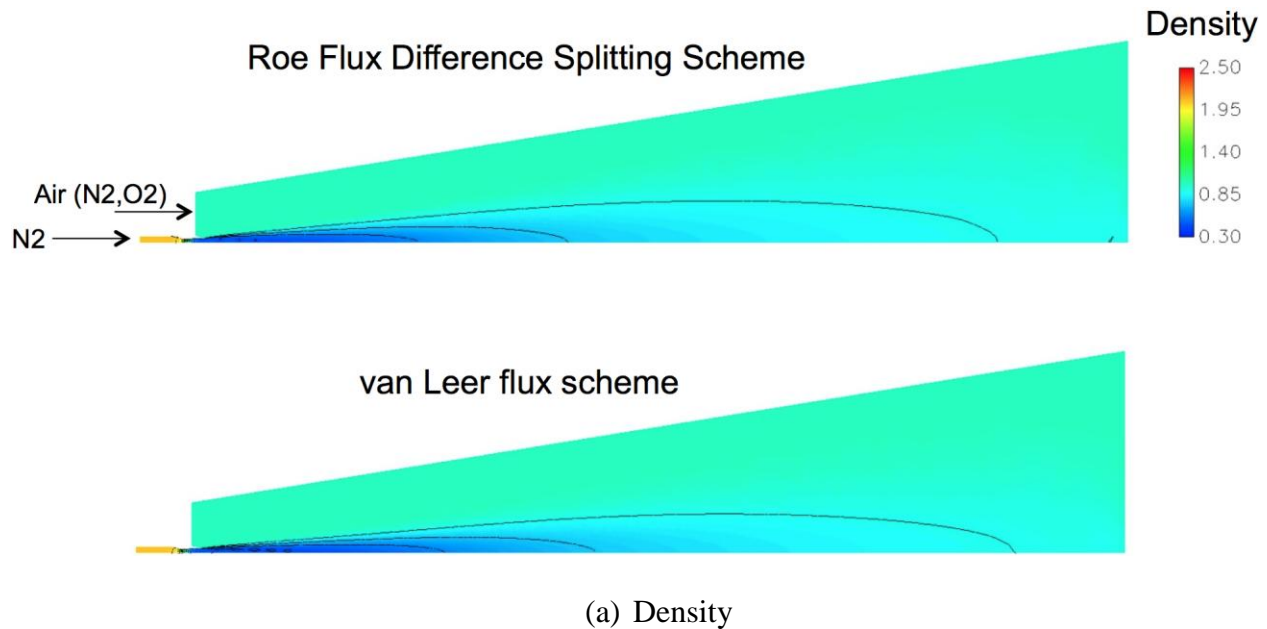


Figure 8.1-1. Comparison of Results from Ideal and Real Air Simulations

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8.2 Comparison of Flux Schemes with N₂ Exhaust Gas

This section presents the comparison of the simulation results using Roe and van Leer flux schemes from the real-gas version of USM3D code. In the following comparison, the ambient gas is taken as a mixture of 73.5 percent N₂ and 26.5 percent O₂. The plenum/nozzle gas is prescribed as 100 percent N₂. The species transport was solved to propagate the species into the domain, along with the energy equation that modifies the ratio of specific heat with temperature. Solutions were started with first-order spatial differencing and switched to second-order. A comparison of density, pressure, temperature, velocity magnitudes, Mach number, and species mass fractions are shown in Figure 8.2-1. The species mass fraction plots show the N₂ mass fraction inside the settling chamber is 1.0, and O₂ mass fraction is zero. It is observed that the distributions of flow variables computed by the Roe scheme and the van Leer scheme are in close agreement, thereby increasing confidence in the implementation of the species transport equations. An expected non-reacting transport of the N₂ species from the engine exhaust into the ambient air was confirmed.





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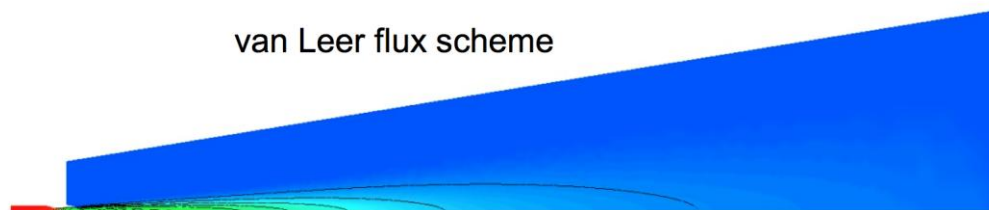
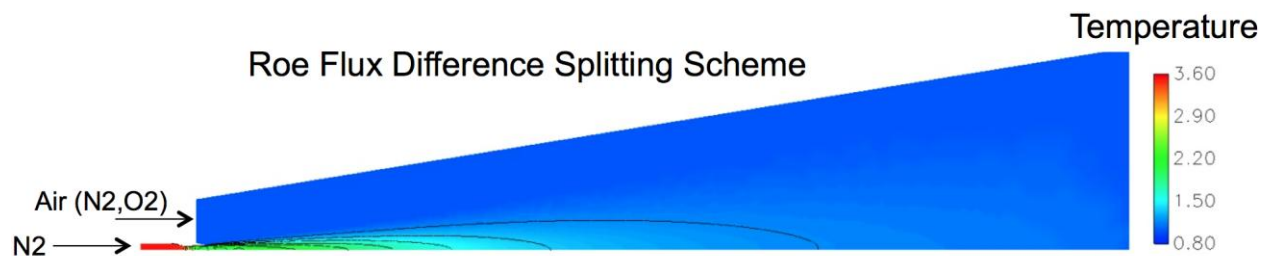
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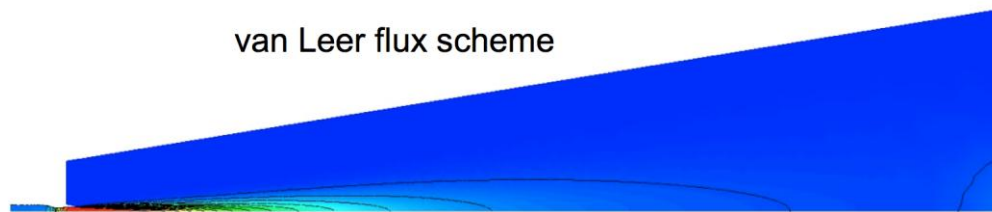
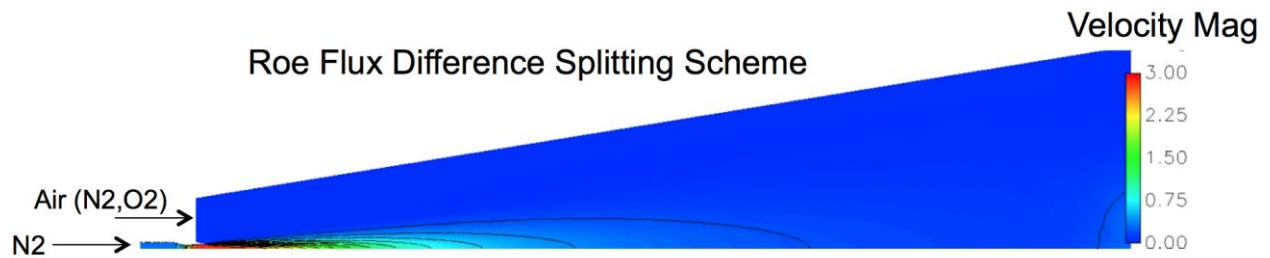
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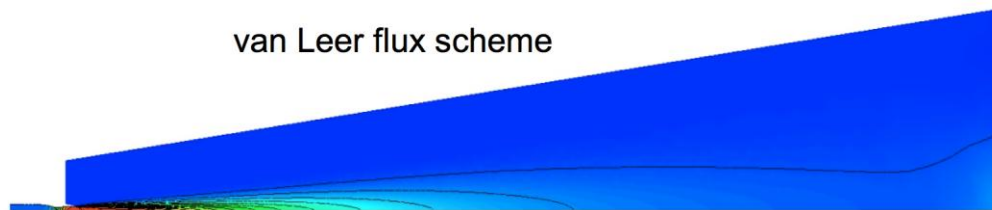
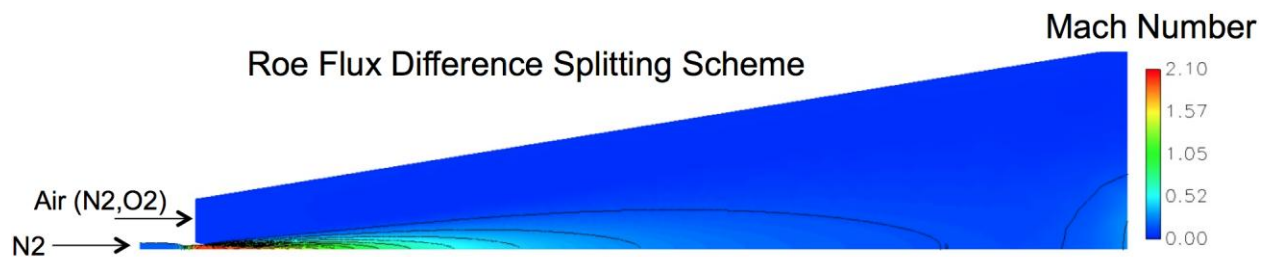
(b) Pressure



(c) Temperature



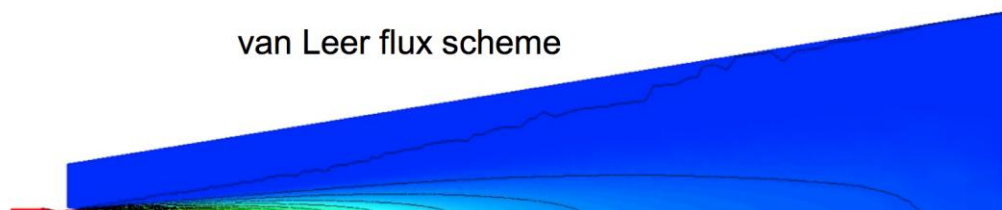
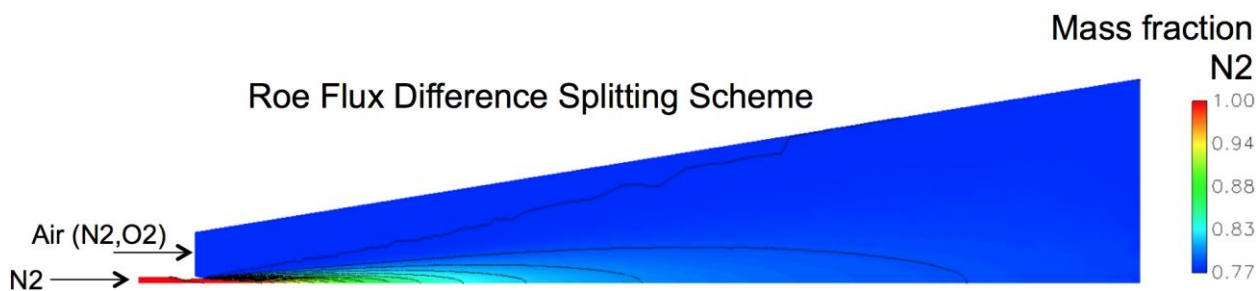
(d) Velocity Magnitude




(e) Mach Number

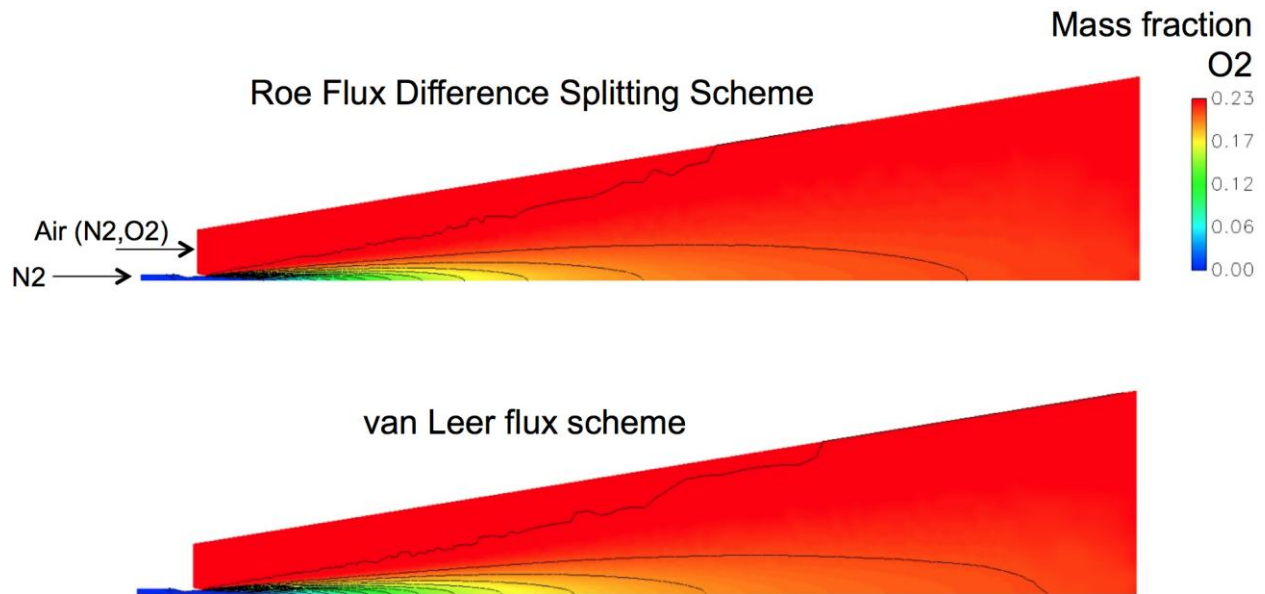


(f) Ratio of Specific Heats



(g) Species Mass fraction: N₂

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(h) Species Mass fraction: O₂

Figure 8.2-1. Results from the Simulations using N₂ as the Exhaust Gas

8.3 Results from Simulations using Hydrogen (H₂) as the Exhaust Gas

This section presents the results from the simulation of the nozzle jet with H₂ as the exhaust gas. With H₂ exhaust gas, the equations are extremely stiff and required more effort to run the simulation. First, the solution was run with first-order differencing with a maximum CFL number of 5. The CFL ramping was set from 1 to 5 over the first 800 iterations. Second, the flow variables inside the plenum were initialized to the hot-gas H₂ conditions to facilitate solution start up. While USM3D has a general capability for modifying prescribed cells, the gas chemistry extension was not added to that feature. For the current testing, the x-coordinate of the cell centroids was used to flag the cells in the plenum and initialize the variables. The number of iterations was set as 30,000, while maintaining the maximum value of CFL number as 5. The distribution of density, pressure, temperature, ratio of specific heats, and species mass fractions after 30,000 iterations are shown in Figure 8.3-1. This figure shows that the flow is not fully developed at the axis of symmetry due to the cell size. Additional iterations are needed to converge the solution and clean up the slight turn in the contour lines near the axis.



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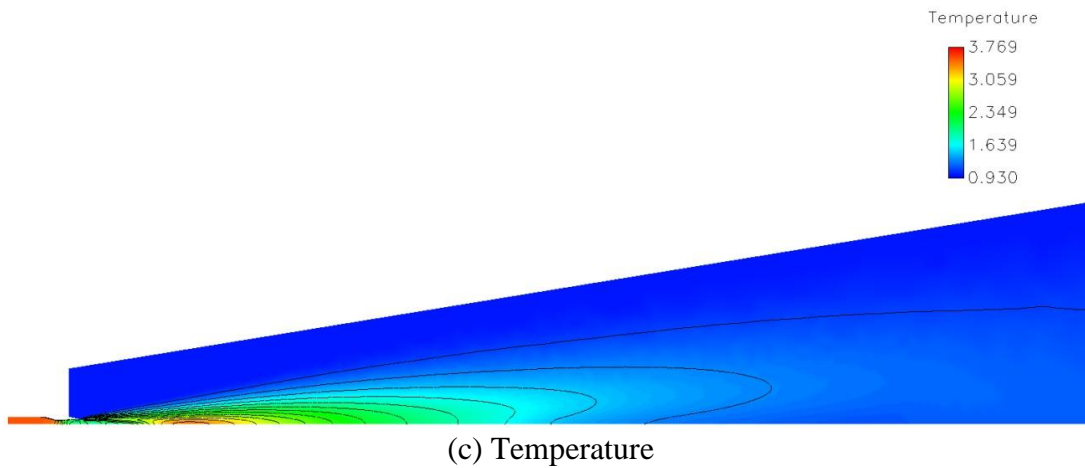
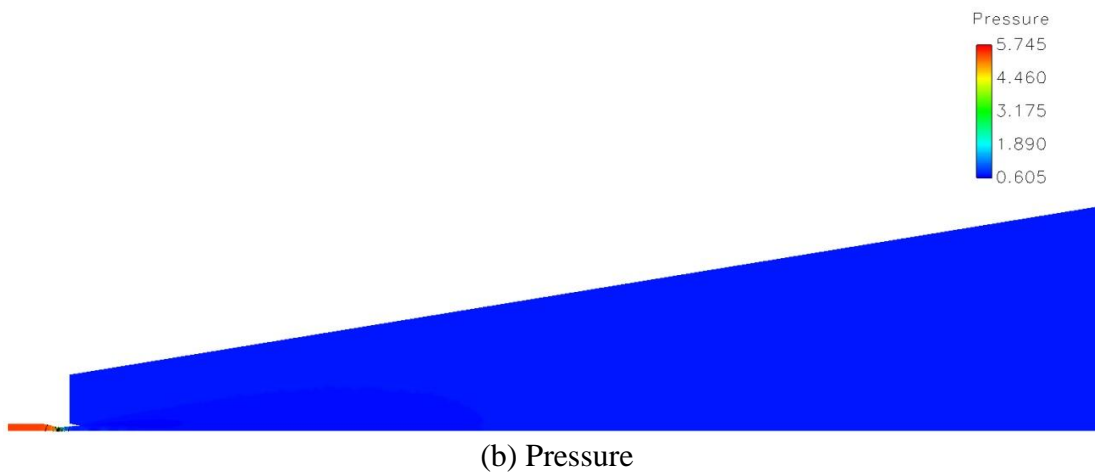
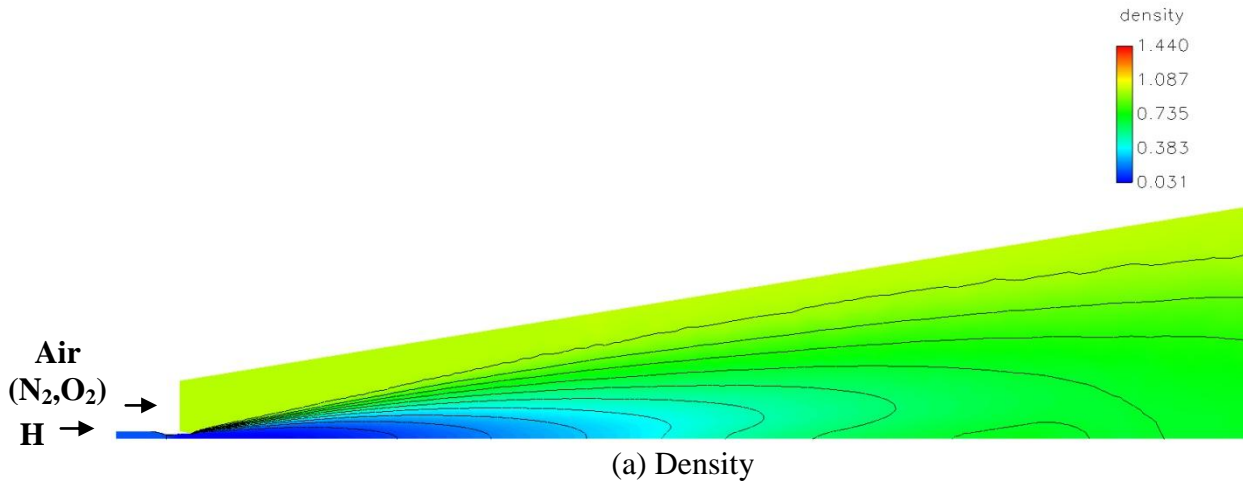
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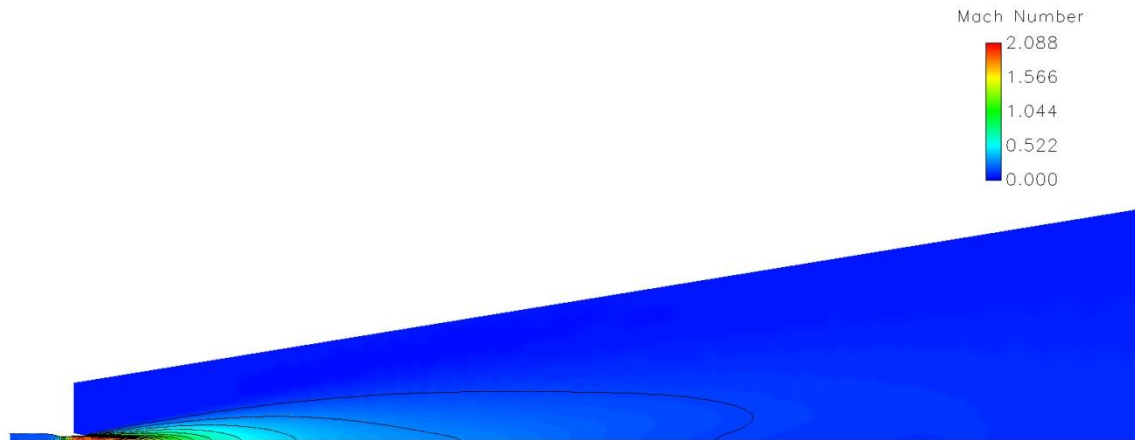
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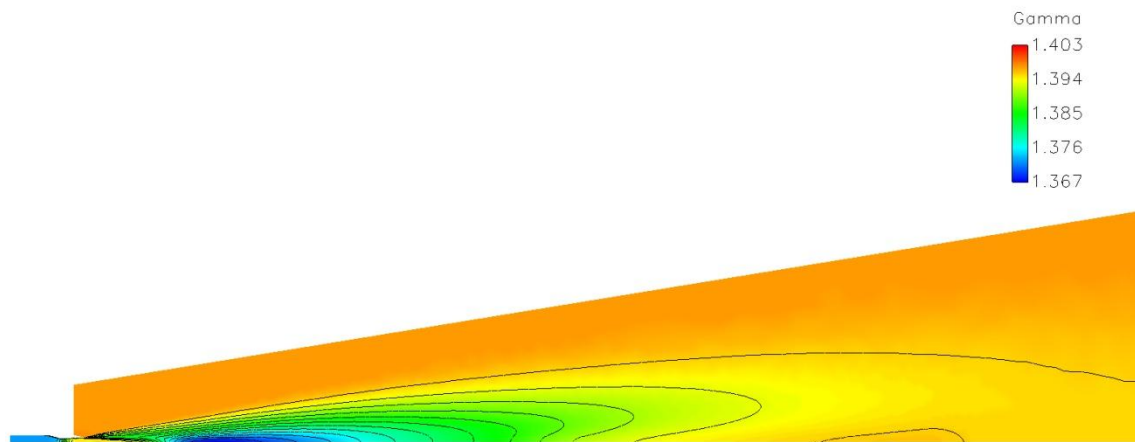
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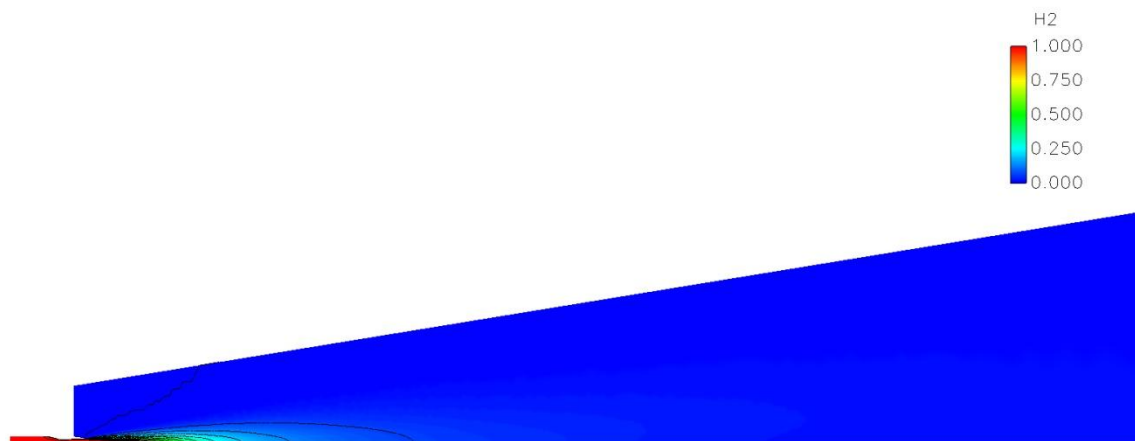
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(d) Mach Number



(e) Ratio of Specific Heats



(f) H₂ Mass Fraction

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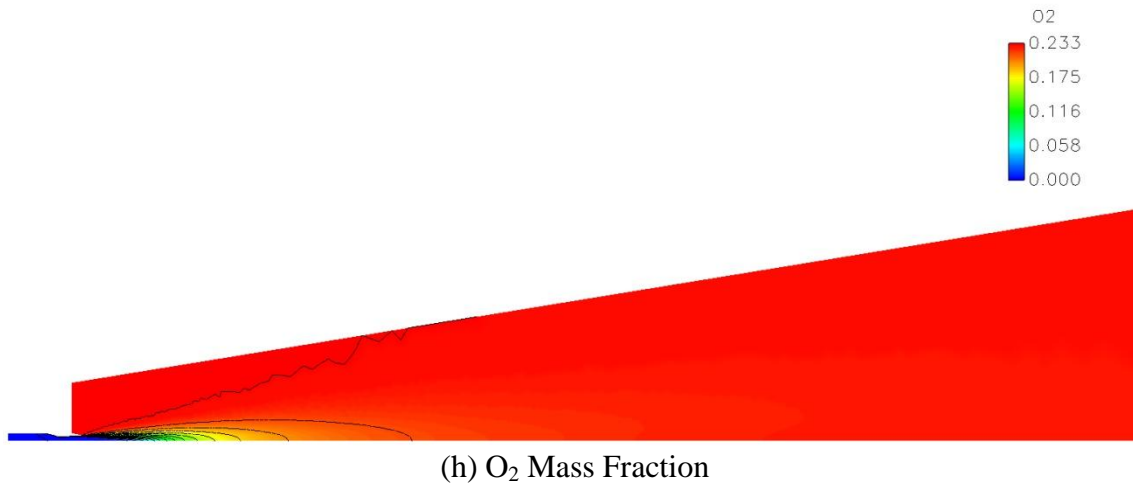
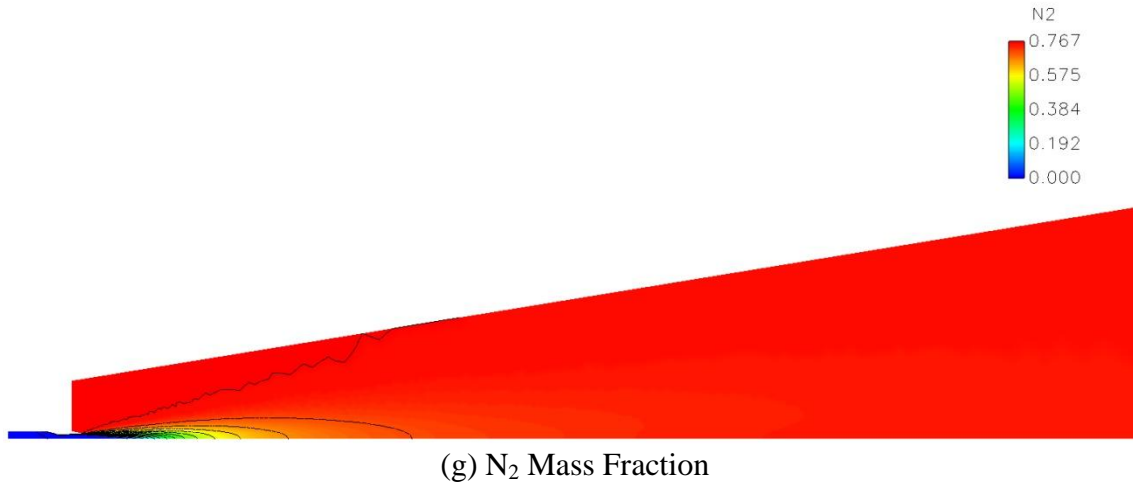


Figure 8.3-1. Results from the Simulations using H₂ as the Exhaust Gas


9.0 Findings, Observations, and NESC Recommendations

9.1 Findings

The following findings were identified:

F-1. The implemented real-gas energy equation solver enables the USM3D code to account for the effect of variable specific heats.

- Solutions require a smaller numerical stability parameter (CFL) to maintain numerical stability, which prolongs run times than its ideal-gas counterpart.

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- F-2.** The van Leer and Roe flux schemes were modified in the USM3D code for real-gas energy equation solver, with the van Leer flux scheme being the most stable.
- F-3.** The species transport equation enables USM3D code to model the multiple species effect.
 - A substantially reduced CFL number is needed to maintain numerical stability. The extent of CFL number reduction depends on the species system.
- F-4.** The numerical modules for solving chemical reactions were developed, but not implemented and tested because of the unresolved numerical stability issues for some multi-species mixing problems.
- F-5.** Continuation of this work is being supported by the SLS Program Aero Task Lead through the services of Dr. Michael Applebaum, Dr. William Eppard, and Mr. Les Hall of CRM Solutions, Inc.

9.2 Observations


The following observations were identified by the Investigators:

- O-1.** The original USM3D flow solver was tightly embedded with the ideal-gas assumption making it difficult to locate every occurrence during the conversion to a real-gas model, thereby increasing the chance for inconsistencies.
- O-2.** Redundancy in the numerical flux scheme coding led to difficulties in implementing a consistent modification for real-gas equations.
- O-3.** The USM3D code has several specialized boundary conditions that presented a challenge to adapt to real-gas formulation.
- O-4.** USM3D uses a one-dimensional array data structure throughout that requires one to have an intimate knowledge of the entire code for making modifications. A more modular approach with locally defined arrays would be desirable.

9.3 NESC Recommendations

The following NESC recommendations are directed to the NASA Technical Fellow for Aerosciences and the Aerothermodynamics Community:

- R-1.** Seek recommendation from CRM Solutions, Inc., on best approach for maturing a robust multi-species and gas chemistry capability in USM3D.
(F-1 through F-5, O-1 through O-4)
- R-2.** Monitor the SLS Program support of the USM3D code modification for application to the MPCV Program crew module launch abort analysis. *(F-5)*

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10.0 Alternate Viewpoints

There were no alternate viewpoints identified during the course of this assessment by the NESC team or the NRB quorum.

11.0 Other Deliverables


There were no other deliverables during the course of this assessment.

12.0 Lessons Learned

No applicable lessons learned were identified for entry into the NASA Lessons Learned Information System.

13.0 Definition of Terms

Corrective Actions	Changes to design processes, work instructions, workmanship practices, training, inspections, tests, procedures, specifications, drawings, tools, equipment, facilities, resources, or material that result in preventing, minimizing, or limiting the potential for recurrence of a problem.
Finding	A conclusion based on facts established by the investigating authority.
Lessons Learned	Knowledge or understanding gained by experience. The experience may be positive, as in a successful test or mission, or negative, as in a mishap or failure. A lesson must be significant in that it has real or assumed impact on operations; valid in that it is factually and technically correct; and applicable in that it identifies a specific design, process, or decision that reduces or limits the potential for failures and mishaps, or reinforces a positive result.
Observation	A factor, event, or circumstance identified during the assessment that did not contribute to the problem, but if left uncorrected has the potential to cause a mishap, injury, or increase the severity should a mishap occur. Alternatively, an observation could be a positive acknowledgement of a Center/Program/Project/Organization's operational structure, tools, and/or support provided.
Problem	The subject of the independent technical assessment.
Proximate Cause	The event(s) that occurred, including any condition(s) that existed immediately before the undesired outcome, directly resulted in its occurrence and, if eliminated or modified, would have prevented the undesired outcome.
Recommendation	An action identified by the NESC to correct a root cause or deficiency identified during the investigation. The recommendations may be used by

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the responsible Center/Program/Project/Organization in the preparation of a corrective action plan.


Root Cause One of multiple factors (events, conditions, or organizational factors) that contributed to or created the proximate cause and subsequent undesired outcome and, if eliminated or modified, would have prevented the undesired outcome. Typically, multiple root causes contribute to an undesired outcome.

14.0 Acronyms List

CFL	Courant-Friedrichs-Lewy
CxP	Constellation Project
H ₂	Hydrogen
LaRC	Langley Research Center
LAV	Launch Abort Vehicle
MPCV	Multi-Purpose Crew Vehicle
N ₂	Nitrogen
NESC	NASA Engineering and Safety Center
NRB	NESC Review Board
O ₂	Oxygen
RCS	Roll Control System
SLS	Space Launch System

14.1 Nomenclature


A	Inviscid flux Jacobian or empirical constant in the Arrhenius form of chemical reaction rate
A_{jk}	Components of the inviscid flux Jacobian
B	Viscous flux Jacobian or empirical constant in the Arrhenius form of chemical reaction rate
B_{jk}	Components of the viscous flux Jacobian
C_p	Specific heat at constant pressure
C_v	Specific heat at constant volume
dV	Elemental volume
dS	Elemental surface area
E	Total energy per unit mass
e	Internal energy per unit mass
E_a	Empirical constant in the Arrhenius form of chemical reaction rate
\vec{F}^i	Inviscid flux vector
$f_1^i, f_2^i, \dots, f_5^i$	Components of inviscid flux vector
\vec{F}^v	Viscous flux vector

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$f_1^v, f_2^v, \dots, f_5^v$	Components of viscous flux vector
h	Enthalpy per unit mass
h_0	Total enthalpy per unit mass
$K_{b,j}$	Backward reaction rate of the j^{th} reaction
$K_{f,j}$	Forward reaction rate of the j^{th} reaction
M_w	Molecular mass
M	Mach number
\vec{n}	Outward pointing unit normal
NR	Number of reactions
NS	Number of species
n_t	Contravariant velocity component of the grid speed and is defined as $n_t = x_t n_x + y_t n_y + z_t n_z$
n_x, n_y, n_z	Components of the unit vector \vec{n}
p	Pressure
Pr	Prandtl number
\vec{Q}	Conserved variable vector
Q_1, Q_2, \dots, Q_5	Components of the conserved variable vector
R	Mixture gas constant
Re	Reynolds number
R_u	Universal gas constant
S	Sutherland constant
T	Temperature
t	Time
u, v, w	Components of velocity in $x, y,$ and z directions, respectively
x_t, y_t, z_t	Components of grids speed in $x, y,$ and z directions, respectively

Greek Letters

α	Species mass fraction defined as the ratio of species density to total density
β	Contravariant velocity component of the fluid particle with respect to the grid and is defined as $\beta = \theta - n_t$
$\Gamma_x, \Gamma_y, \Gamma_z$	Geometric factors
κ	Coefficient of thermal conductivity and is defined as $\kappa = \frac{C_p \mu}{Pr}$
γ	Ratio of specific heats
ρ	Density
μ	Dynamic viscosity
$\dot{\omega}$	Source term due to chemical reaction

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θ Contravariant velocity component of the fluid particle and is defined as

$$\theta = un_x + vn_y + wn_z$$

ν Stoichiometric coefficient

$\tau_{xx}, \tau_{xy}, \tau_{xz}, \tau_{yy}, \tau_{yz}, \tau_{zz}$ Component of the rate of shear stress tensor

Subscripts

b Backward reaction

f Forward reaction

ref Reference conditions

s Species index

x, y, z Components of a vector along $x, y,$ and z directions, respectively

∞ Freestream conditions

Over

\wedge Dimensional quantities

\rightarrow Vectors

\Rightarrow Tensors

15.0 References

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16.0 Appendices


Appendix A. Derivation of Inviscid and Viscous Jacobians

Appendix B. Linearization of Pressure for Real Gases

Appendix C. Numerical Treatment of Characteristic Boundary Conditions in Subroutine UBC2

Appendix D. Numerical Treatment of Viscous Wall Boundary Conditions

Appendix E. Description of USM3D Input File

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Appendix A. Derivation of Inviscid and Viscous Jacobians

Representing the conserved variable vector Q as:

$$\vec{Q} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \\ Q_5 \end{bmatrix} \quad (\text{A.1})$$

The contravariant velocity can be represented as:

$$\theta = \frac{1}{Q_1} (Q_2 n_x + Q_3 n_y + Q_4 n_z) \quad (\text{A.2})$$

Using Equation (5), the inviscid flux vector can be written as:

$$\vec{F}^i \cdot \vec{n} = \begin{bmatrix} f_1^i \\ f_2^i \\ f_3^i \\ f_4^i \\ f_5^i \end{bmatrix} = \begin{bmatrix} -n_x Q_1 + n_x Q_2 + n_y Q_3 + n_y Q_4 \\ \frac{Q_2}{Q_1} (-n_x Q_1 + n_x Q_2 + n_y Q_3 + n_y Q_4) + n_x p \\ \frac{Q_3}{Q_1} (-n_x Q_1 + n_x Q_2 + n_y Q_3 + n_y Q_4) + n_y p \\ \frac{Q_4}{Q_1} (-n_x Q_1 + n_x Q_2 + n_y Q_3 + n_y Q_4) + n_z p \\ \frac{Q_5}{Q_1} (-n_x Q_1 + n_x Q_2 + n_y Q_3 + n_y Q_4) + \frac{p}{Q_1} (n_x Q_2 + n_y Q_3 + n_y Q_4) \end{bmatrix} \quad (\text{A.3})$$

Equation (A.3) can be differentiated with respect to A.1 to get the inviscid flux Jacobian. Each component of the inviscid flux vector can be represented as $A_{jk} = \frac{\partial f_j^i}{\partial Q_k}$ and this will result in:

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{bmatrix} \quad (\text{A.4})$$



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$$A = \begin{bmatrix} -n_t & n_x & n_y & n_z & 0 \\ n_x \phi - u \theta & n_x(2-\gamma)u + U & n_y u - n_x(\gamma-1)v & n_z u - n_x(\gamma-1)w & n_x(\gamma-1) \\ n_y \phi - v \theta & n_x v - n_y(\gamma-1)u & n_y(2-\gamma)v + U & n_z v - n_y(\gamma-1)w & n_y(\gamma-1) \\ n_z \phi - w \theta & n_x w - n_z(\gamma-1)u & n_y w - n_z(\gamma-1)v & n_z(2-\gamma)w + U & n_z(\gamma-1) \\ \left(2\phi - \frac{\gamma E}{\rho}\right)\theta & n_x \left(\frac{\gamma E}{\rho} - \phi\right) - (\gamma-1)u\theta & n_y \left(\frac{\gamma E}{\rho} - \phi\right) - (\gamma-1)v\theta & n_z \left(\frac{\gamma E}{\rho} - \phi\right) - (\gamma-1)w\theta & \gamma\theta - n_t \end{bmatrix}$$

and

$$A_{11} = \frac{\partial f_1^i}{\partial Q_1} = -n_t; \quad A_{12} = \frac{\partial f_1^i}{\partial Q_2} = n_x; \quad A_{13} = \frac{\partial f_1^i}{\partial Q_3} = n_y; \quad A_{14} = \frac{\partial f_1^i}{\partial Q_4} = n_z; \quad A_{15} = \frac{\partial f_1^i}{\partial Q_5} = 0$$

$$A_{21} = \frac{\partial f_2^i}{\partial Q_1} = \frac{\partial}{\partial Q_1} \left(-n_t Q_2 + n_x \frac{Q_2^2}{Q_1} + n_y \frac{Q_2 Q_3}{Q_1} + n_z \frac{Q_2 Q_4}{Q_1} + n_x p \right) = -\frac{Q_2}{Q_1} \theta + n_x \frac{\partial p}{\partial \rho}$$

$$A_{22} = \frac{\partial f_2^i}{\partial Q_2} = \beta + n_x(2-\gamma) \frac{Q_2}{Q_1}$$

$$A_{23} = \frac{\partial f_2^i}{\partial Q_3} = n_y \frac{Q_2}{Q_1} - n_x(\gamma-1) \frac{Q_3}{Q_1}$$

$$A_{24} = \frac{\partial f_2^i}{\partial Q_4} = n_z \frac{Q_2}{Q_1} - n_x(\gamma-1) \frac{Q_4}{Q_1}$$

$$A_{25} = \frac{\partial f_2^i}{\partial Q_5} = n_x(\gamma-1)$$

$$A_{31} = \frac{\partial f_3^i}{\partial Q_1} = \frac{\partial}{\partial Q_1} \left(-n_t Q_3 + n_x \frac{Q_2 Q_3}{Q_1} + n_y \frac{Q_3^2}{Q_1} + n_z \frac{Q_3 Q_4}{Q_1} + n_y p \right) = -\frac{Q_3}{Q_1} \theta + n_y \frac{\partial p}{\partial \rho}$$

$$A_{32} = \frac{\partial f_3^i}{\partial Q_2} = n_x \frac{Q_3}{Q_1} - n_y(\gamma-1) \frac{Q_2}{Q_1}$$

$$A_{33} = \frac{\partial f_3^i}{\partial Q_3} = \beta + n_y(2-\gamma) \frac{Q_3}{Q_1}$$

$$A_{34} = \frac{\partial f_3^i}{\partial Q_4} = n_z \frac{Q_3}{Q_1} - n_y(\gamma-1) \frac{Q_4}{Q_1}$$

$$A_{35} = \frac{\partial f_3^i}{\partial Q_5} = n_y(\gamma-1)$$



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$$A_{41} = \frac{\partial f_4^i}{\partial Q_1} = \frac{\partial}{\partial Q_1} \left(-n_t Q_4 + n_x \frac{Q_2 Q_4}{Q_1} + n_y \frac{Q_3 Q_4}{Q_1} + n_z \frac{Q_4^2}{Q_1} + n_z p \right) = -\frac{Q_4}{Q_1} \theta + n_z \frac{\partial p}{\partial \rho}$$

$$A_{42} = \frac{\partial f_4^i}{\partial Q_2} = n_x \frac{Q_4}{Q_1} - n_z (\gamma - 1) \frac{Q_2}{Q_1}$$

$$A_{43} = \frac{\partial f_4^i}{\partial Q_3} = n_y \frac{Q_4}{Q_1} - n_z (\gamma - 1) \frac{Q_3}{Q_1}$$

$$A_{44} = \frac{\partial f_4^i}{\partial Q_4} = \beta + n_z (2 - \gamma) \frac{Q_4}{Q_1}$$

$$A_{45} = \frac{\partial f_4^i}{\partial Q_5} = n_z (\gamma - 1)$$

$$A_{51} = \frac{\partial f_5^i}{\partial Q_1} = \frac{\partial}{\partial Q_1} \left(-n_t Q_5 + n_x \frac{Q_2 Q_5}{Q_1} + n_y \frac{Q_3 Q_5}{Q_1} + n_z \frac{Q_4 Q_5}{Q_1} + n_x p \frac{Q_2}{Q_1} + n_y p \frac{Q_3}{Q_1} + n_z p \frac{Q_4}{Q_1} \right)$$
$$= \theta \left[-\gamma \frac{Q_5}{Q_1} + \frac{\gamma - 1}{Q_1} (Q_2^2 + Q_3^2 + Q_4^2) \right]$$

$$A_{52} = \frac{\partial f_5^i}{\partial Q_2} = n_x \frac{Q_5 + p}{Q_1} - \theta (\gamma - 1) \frac{Q_2}{Q_1}$$


$$A_{53} = \frac{\partial f_5^i}{\partial Q_3} = n_y \frac{Q_5 + p}{Q_1} - \theta (\gamma - 1) \frac{Q_3}{Q_1}$$

$$A_{54} = \frac{\partial f_5^i}{\partial Q_4} = n_z \frac{Q_5 + p}{Q_1} - \theta (\gamma - 1) \frac{Q_4}{Q_1}$$

$$A_{55} = \frac{\partial f_5^i}{\partial Q_5} = \gamma \theta - n_t$$

where $\frac{\partial p}{\partial \rho} = \frac{p}{Q_1} + \frac{\gamma - 1}{Q_1} (-Q_5 + Q_2^2 + Q_3^2 + Q_4^2)$ is derived as shown in Appendix B. For constant specific heat assumption:

$$\frac{\partial p}{\partial \rho} = \frac{\gamma - 1}{2 Q_1} (Q_2^2 + Q_3^2 + Q_4^2) = \frac{\gamma - 1}{2} (u^2 + v^2 + w^2)$$

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Also, representing the dependent variable vector q as:

$$\bar{q} = \begin{bmatrix} \rho \\ u \\ v \\ w \\ p \end{bmatrix} = \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2/Q_1 \\ Q_3/Q_1 \\ Q_4/Q_1 \\ q_5 \end{bmatrix}$$

Hence,

$$\frac{\partial \bar{q}}{\partial \bar{Q}} = \begin{bmatrix} \frac{\partial q_1}{\partial Q_1} & \frac{\partial q_1}{\partial Q_2} & \frac{\partial q_1}{\partial Q_3} & \frac{\partial q_1}{\partial Q_4} & \frac{\partial q_1}{\partial Q_5} \\ \frac{\partial q_2}{\partial Q_1} & \frac{\partial q_2}{\partial Q_2} & \frac{\partial q_2}{\partial Q_3} & \frac{\partial q_2}{\partial Q_4} & \frac{\partial q_2}{\partial Q_5} \\ \frac{\partial q_3}{\partial Q_1} & \frac{\partial q_3}{\partial Q_2} & \frac{\partial q_3}{\partial Q_3} & \frac{\partial q_3}{\partial Q_4} & \frac{\partial q_3}{\partial Q_5} \\ \frac{\partial q_4}{\partial Q_1} & \frac{\partial q_4}{\partial Q_2} & \frac{\partial q_4}{\partial Q_3} & \frac{\partial q_4}{\partial Q_4} & \frac{\partial q_4}{\partial Q_5} \\ \frac{\partial q_5}{\partial Q_1} & \frac{\partial q_5}{\partial Q_2} & \frac{\partial q_5}{\partial Q_3} & \frac{\partial q_5}{\partial Q_4} & \frac{\partial q_5}{\partial Q_5} \end{bmatrix}$$


$$\frac{\partial \bar{q}}{\partial \bar{Q}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -u/\rho & 1/\rho & 0 & 0 & 0 \\ -v/\rho & 0 & 1/\rho & 0 & 0 \\ -w/\rho & 0 & 0 & 1/\rho & 0 \\ \frac{\partial p}{\partial \rho} & -(\gamma-1)u & -(\gamma-1)v & -(\gamma-1)w & \gamma-1 \end{bmatrix}$$

where:

$$\frac{\partial q_1}{\partial Q_1} = \frac{\partial Q_1}{\partial Q_1} = 1; \quad \frac{\partial q_1}{\partial Q_2} = \frac{\partial q_1}{\partial Q_3} = \frac{\partial q_1}{\partial Q_4} = \frac{\partial q_1}{\partial Q_5} = 0$$

$$\frac{\partial q_2}{\partial Q_1} = \frac{\partial Q_2/Q_1}{\partial Q_1} = -\frac{Q_2}{Q_1^2} = \frac{-u}{\rho}; \quad \frac{\partial q_2}{\partial Q_2} = \frac{\partial Q_2/Q_1}{\partial Q_2} = \frac{1}{Q_1} = \frac{1}{\rho}; \quad \frac{\partial q_2}{\partial Q_3} = \frac{\partial q_2}{\partial Q_4} = \frac{\partial q_2}{\partial Q_5} = 0$$

$$\frac{\partial q_3}{\partial Q_1} = \frac{\partial Q_3/Q_1}{\partial Q_1} = -\frac{Q_3}{Q_1^2} = \frac{-v}{\rho}; \quad \frac{\partial q_3}{\partial Q_3} = \frac{\partial Q_3/Q_1}{\partial Q_3} = \frac{1}{Q_1} = \frac{1}{\rho}; \quad \frac{\partial q_3}{\partial Q_2} = \frac{\partial q_3}{\partial Q_4} = \frac{\partial q_3}{\partial Q_5} = 0$$

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$$\frac{\partial q_4}{\partial Q_1} = \frac{\partial Q_4/Q_1}{\partial Q_1} = -\frac{Q_4}{Q_1^2} = -\frac{w}{\rho}; \quad \frac{\partial q_4}{\partial Q_4} = \frac{\partial Q_4/Q_1}{\partial Q_4} = \frac{1}{Q_1} = \frac{1}{\rho}; \quad \frac{\partial q_4}{\partial Q_2} = \frac{\partial q_4}{\partial Q_3} = \frac{\partial q_4}{\partial Q_5} = 0$$

And $\partial q_5/\partial Q_1$, $\partial q_5/\partial Q_2$, $\partial q_5/\partial Q_3$, $\partial q_5/\partial Q_4$, $\partial q_5/\partial Q_5$ can be obtained as shown in Appendix B and shown as the following:

$$\frac{\partial q_5}{\partial Q_1} = \frac{\partial P}{\partial \rho} = \frac{\gamma-1}{Q_1} \left(\frac{P}{\gamma-1} - Q_5 + Q_2^2 + Q_3^2 + Q_4^2 \right)$$

$$\frac{\partial q_5}{\partial Q_2} = -(\gamma-1)u = -(\gamma-1)\frac{Q_2}{Q_1}$$

$$\frac{\partial q_5}{\partial Q_3} = -(\gamma-1)v = -(\gamma-1)\frac{Q_3}{Q_1}$$

$$\frac{\partial q_5}{\partial Q_4} = -(\gamma-1)w = -(\gamma-1)\frac{Q_4}{Q_1}$$

$$\frac{\partial q_5}{\partial Q_5} = \gamma-1$$

Hence,


$$\frac{\partial \vec{q}}{\partial \vec{Q}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -u/\rho & 1/\rho & 0 & 0 & 0 \\ -v/\rho & 0 & 1/\rho & 0 & 0 \\ -w/\rho & 0 & 0 & 1/\rho & 0 \\ \frac{\partial P}{\partial \rho} & -(\gamma-1)u & -(\gamma-1)v & -(\gamma-1)w & \gamma-1 \end{bmatrix} \quad (\text{A.5})$$

From Equation 14, the team can obtain:

$$dT = -\frac{T}{\rho} d\rho + \frac{\gamma_{\text{ref}}}{\rho R} dp$$

Hence,

$$\frac{\partial T}{\partial \vec{q}} = \begin{bmatrix} -\frac{T}{\rho} & 0 & 0 & 0 & \frac{\gamma_{\text{ref}}}{\rho R} \end{bmatrix} \quad (\text{A.6})$$

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Combine Equations (A.5) and (A.6), the team can obtain:

$$\begin{aligned}
 \frac{\partial T}{\partial \bar{Q}} &= \left[\frac{\partial T}{\partial Q_1} \quad \frac{\partial T}{\partial Q_2} \quad \frac{\partial T}{\partial Q_3} \quad \frac{\partial T}{\partial Q_4} \quad \frac{\partial T}{\partial Q_5} \right] = \frac{\partial T}{\partial \bar{q}} \frac{\partial \bar{q}}{\partial \bar{Q}} \\
 &= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -u/\rho & 1/\rho & 0 & 0 & 0 \\ -v/\rho & 0 & 1/\rho & 0 & 0 \\ -w/\rho & 0 & 0 & 1/\rho & 0 \\ \frac{\partial p}{\partial \rho} & -(\gamma-1)u & -(\gamma-1)v & -(\gamma-1)w & \gamma-1 \end{bmatrix} \\
 &= \begin{bmatrix} -T/\rho & 0 & 0 & 0 & \gamma_{\text{ref}}/\rho R \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -u/\rho & 1/\rho & 0 & 0 & 0 \\ -v/\rho & 0 & 1/\rho & 0 & 0 \\ -w/\rho & 0 & 0 & 1/\rho & 0 \\ \frac{\partial p}{\partial \rho} & -(\gamma-1)u & -(\gamma-1)v & -(\gamma-1)w & \gamma-1 \end{bmatrix} \\
 &= \begin{bmatrix} -T/\rho + \frac{\gamma_{\text{ref}}}{\rho R} \frac{\partial p}{\partial \rho} & \frac{-\gamma_{\text{ref}}(\gamma-1)u}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)v}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)w}{\rho R} & \frac{\gamma_{\text{ref}}(\gamma-1)}{\rho R} \end{bmatrix} \\
 &= \begin{bmatrix} -T/\rho + \frac{\gamma_{\text{ref}}}{\rho R} \frac{(\gamma-1)V^2}{2} & \frac{-\gamma_{\text{ref}}(\gamma-1)u}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)v}{\rho R} & \frac{-\gamma_{\text{ref}}(\gamma-1)w}{\rho R} & \frac{\gamma_{\text{ref}}(\gamma-1)}{\rho R} \end{bmatrix}
 \end{aligned} \tag{A.7}$$

The spatial derivatives a dependent variable ϕ at the interface between two adjacent cells can be calculated as:

$$\begin{aligned}
 \phi_x &= \frac{\partial \phi}{\partial x} = \Gamma_x \Delta \phi; \quad \Gamma_x = \frac{n_x}{n_x \Delta x + n_y \Delta y + n_z \Delta z} \\
 \phi_y &= \frac{\partial \phi}{\partial y} = \Gamma_y \Delta \phi; \quad \Gamma_y = \frac{n_y}{n_x \Delta x + n_y \Delta y + n_z \Delta z} \\
 \phi_z &= \frac{\partial \phi}{\partial z} = \Gamma_z \Delta \phi; \quad \Gamma_z = \frac{n_z}{n_x \Delta x + n_y \Delta y + n_z \Delta z}
 \end{aligned}$$

and $\Delta \phi = \phi_R - \phi_L$ where ϕ_R and ϕ_L are the values of ϕ at the center of right and left. Hence, the spatial derivatives of a dependent variable at the cell face can be linearized by the conservative \bar{Q} as:

$$\frac{\partial \phi_x}{\partial \bar{Q}} = \Gamma_x \frac{\partial(\Delta \phi)}{\partial \bar{Q}} = \Gamma_x \left(\frac{\partial(\phi_R - \phi_L)}{\partial \bar{Q}} \right) \tag{A.8}$$

Therefore,

$$\frac{\partial \phi_x}{\partial \bar{Q}_R} = \Gamma_x \left(\frac{\partial \phi_R}{\partial \bar{Q}_R} \right)$$



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$$\frac{\partial \phi_x}{\partial \bar{Q}_L} = -\Gamma_x \left(\frac{\partial \phi_L}{\partial \bar{Q}_L} \right)$$

Equation (13) can be differentiated with respect to (A.1) to get the viscous flux Jacobian. Each component of the viscous flux vector can be represented as $B_{jk} = \frac{\partial f_j^v}{\partial Q_k}$ and this will result in:

$$B = \begin{bmatrix} B_{11} & B_{12} & B_{13} & B_{14} & B_{15} \\ B_{21} & B_{22} & B_{23} & B_{24} & B_{25} \\ B_{31} & B_{32} & B_{33} & B_{34} & B_{35} \\ B_{41} & B_{42} & B_{43} & B_{44} & B_{45} \\ B_{51} & B_{52} & B_{53} & B_{54} & B_{55} \end{bmatrix} \quad (\text{A.9})$$

Substituting Equations (A.8), (A.10), and (A.11), each components of the viscous flux Jacobian can be expressed as:

$$B_{11} = B_{12} = B_{13} = B_{14} = B_{15} = 0$$

$$B_{2j} = \frac{\partial f_2^v}{\partial (Q_c)_j} = \left(n_x \frac{\partial \tau_{xx}}{\partial (Q_c)_j} + n_y \frac{\partial \tau_{yx}}{\partial (Q_c)_j} + n_z \frac{\partial \tau_{zx}}{\partial (Q_c)_j} \right)$$


$$B_{3j} = \frac{\partial f_3^v}{\partial (Q_c)_j} = \left(n_x \frac{\partial \tau_{xy}}{\partial (Q_c)_j} + n_y \frac{\partial \tau_{yy}}{\partial (Q_c)_j} + n_z \frac{\partial \tau_{zy}}{\partial (Q_c)_j} \right)$$

$$B_{4j} = \frac{\partial f_4^v}{\partial (Q_c)_j} = \left(n_x \frac{\partial \tau_{xz}}{\partial (Q_c)_j} + n_y \frac{\partial \tau_{yz}}{\partial (Q_c)_j} + n_z \frac{\partial \tau_{zz}}{\partial (Q_c)_j} \right)$$

$$B_{5j} = \frac{\partial f_5^v}{\partial (Q_c)_j} = \frac{\partial (u_f f_2^v)}{\partial (Q_c)_j} + \frac{\partial (v_f f_3^v)}{\partial (Q_c)_j} + \frac{\partial (w_f f_4^v)}{\partial (Q_c)_j} + \kappa \left(n_x \frac{\partial T_x}{\partial (Q_c)_j} + n_y \frac{\partial T_y}{\partial (Q_c)_j} + n_z \frac{\partial T_z}{\partial (Q_c)_j} \right)$$

$$= u_f B_{2j} + v_f B_{3j} + w_f B_{4j} + \kappa \left(n_x \frac{\partial T_x}{\partial (Q_c)_j} + n_y \frac{\partial T_y}{\partial (Q_c)_j} + n_z \frac{\partial T_z}{\partial (Q_c)_j} \right)$$

where C represents either cell on the left or cell on the right side of the face and j represents the column number.

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Appendix B. Linearization of Pressure for Real Gases

For thermally perfect, single-species flow:

$$p = \frac{\rho RT}{\gamma_{\text{ref}}}$$

Hence,

$$dp = \frac{RT}{\gamma_{\text{ref}}} d\rho + \frac{\rho R}{\gamma_{\text{ref}}} dT \quad (\text{B.1})$$

Since the specific internal energy (e) is defined as:

$$de = \frac{C_v}{\gamma_{\text{ref}}} dT \Rightarrow \frac{1}{\gamma_{\text{ref}}} dT = \frac{de}{C_v} \quad (\text{B.2})$$

Also, the specific total energy (E) is defined as:

$$E = e + \frac{1}{2}(u^2 + v^2 + w^2)$$

Hence,

$$dE = de + udu + vdv + wdw, \text{ or } de = dE - (udu + vdv + wdw) \quad (\text{B.3})$$

For a general flow variable Φ

$$d(\rho\Phi) = \rho d\Phi + \Phi d\rho \Rightarrow d\Phi = \frac{d(\rho\Phi) - \Phi d\rho}{\rho}$$

Apply the above equation for flow variables, E , u , v , and w to Eq. (B.3), the team can obtain:

$$de = \frac{d(\rho E) - E d\rho + (u^2 + v^2 + w^2) d\rho - [u d(\rho u) + v d(\rho v) + w d(\rho w)]}{\rho} \quad (\text{B.4})$$

Substitute Equation (B.4) into Equation (B.2):

$$\frac{1}{\gamma_{\text{ref}}} dT = \frac{d(\rho E) - E d\rho + (u^2 + v^2 + w^2) d\rho - [u d(\rho u) + v d(\rho v) + w d(\rho w)]}{\rho C_v} \quad (\text{B.5})$$

Substitute Equation (B.5) into Equation (B.1), the team can obtain:



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$$\begin{aligned}
 dp &= RTd\rho + \frac{R}{C_v} \left\{ d(\rho E) - Ed\rho + (u^2 + v^2 + w^2)d\rho - [ud(\rho u) + vd(\rho v) + wd(\rho w)] \right\} \\
 &= \frac{R}{C_v} \left[\left(\frac{C_v T}{\gamma_{\text{ref}}} - E + u^2 + v^2 + w^2 \right) d\rho - ud(\rho u) - vd(\rho v) - wd(\rho w) + d(\rho E) \right] \\
 &= (\gamma - 1) \left(\frac{P}{(\gamma - 1)\rho} - E + u^2 + v^2 + w^2 \right) d\rho - (\gamma - 1)ud(\rho u) - (\gamma - 1)vd(\rho v) \\
 &\quad - (\gamma - 1)wd(\rho w) + (\gamma - 1)d(\rho E) \\
 &= \frac{\partial p}{\partial Q_1} dQ_1 + \frac{\partial p}{\partial Q_2} dQ_2 + \frac{\partial p}{\partial Q_3} dQ_3 + \frac{\partial p}{\partial Q_4} dQ_4 + \frac{\partial p}{\partial Q_5} dQ_5
 \end{aligned} \tag{B.6}$$

where

$$\vec{Q} = \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \\ Q_5 \end{bmatrix} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix}$$

and

$$\begin{aligned}
 \frac{\partial p}{\partial Q_1} &= (\gamma - 1) \left(\frac{P}{(\gamma - 1)\rho} - E + u^2 + v^2 + w^2 \right) = \frac{P}{Q_1} + \frac{\gamma - 1}{Q_1} (-Q_5 + Q_2^2 + Q_3^2 + Q_4^2) = \frac{\partial p}{\partial \rho} \\
 \frac{\partial p}{\partial Q_2} &= -(\gamma - 1)u = -(\gamma - 1) \frac{Q_2}{Q_1} \\
 \frac{\partial p}{\partial Q_3} &= -(\gamma - 1)v = -(\gamma - 1) \frac{Q_3}{Q_1} \\
 \frac{\partial p}{\partial Q_4} &= -(\gamma - 1)w = -(\gamma - 1) \frac{Q_4}{Q_1} \\
 \frac{\partial p}{\partial Q_5} &= \gamma - 1
 \end{aligned} \tag{B.7}$$

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Appendix C. Numerical Treatment of Characteristic Boundary Conditions in Subroutine UBC2

Current formulation (constant $\gamma = \gamma_\infty$):

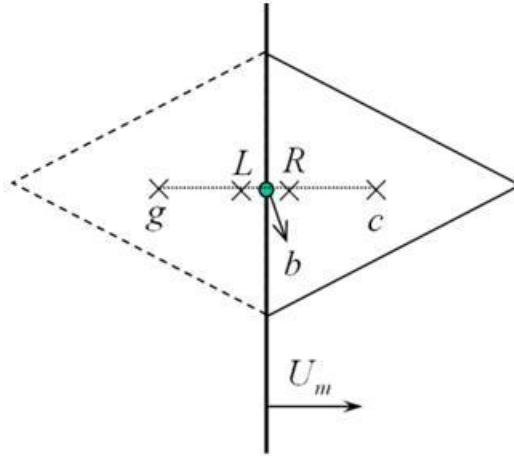


Figure C-1. Orientation of Boundary Face for Characteristic Variable based Boundary Condition

Based on the orientation of a boundary face and the nomenclature used in Figure C-1, the Riemann invariants can be written as:

$$\mathfrak{R}^+ = U_R + \frac{2a_R}{\gamma - 1} = U_b + \frac{2a_b}{\gamma - 1}$$

$$\mathfrak{R}^- = U_L + \frac{2a_L}{\gamma - 1} = U_b - \frac{2a_b}{\gamma - 1}$$


where U and a are the contravariant velocity and speed of sound, and

$$U_R = U_c + \nabla U \cdot \Delta \vec{s}; \quad U_L = U_g = U_\infty$$

Subscript ∞ denote the freestream condition. Hence, the condition at the boundary can be obtained as:

$$U_b = \frac{1}{2}(\mathfrak{R}^+ + \mathfrak{R}^-); \quad a_b = \frac{\gamma - 1}{4}(\mathfrak{R}^+ - \mathfrak{R}^-)$$

If $U_b + U_m \geq 0$ where U_m is the contravariant velocity of the moving boundary, then the information is traveling from the right-hand-side. Hence,

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$$\begin{aligned}
 u_b &= u_R + n_x(U_b - U_R) \\
 v_b &= v_R + n_y(U_b - U_R) \\
 w_b &= w_R + n_z(U_b - U_R)
 \end{aligned}$$

To obtain the thermal properties at the boundary, isentropic process between R and b is assumed, and thus

$$\frac{T_b}{\rho_b^{\gamma-1}} = \frac{T_R}{\rho_R^{\gamma-1}} \Rightarrow \rho_b = \left[\frac{T_b}{T_R / \rho_R^{\gamma-1}} \right]^{\frac{1}{\gamma-1}} \quad \text{and} \quad p_b = \frac{1}{\gamma} \rho_b T_b$$

where

$$T_b = a_b^2; \quad T_R = \gamma \frac{p_R}{\rho_R}; \quad p_R = p_c + \nabla p \cdot \Delta \vec{s}; \quad \rho_R = \rho_c + \nabla \rho \cdot \Delta \vec{s}$$

If $U_b + U_m < 0$, then the information is traveling from the left-hand-side. Hence,

$$\begin{aligned}
 u_b &= u_L + n_x(U_b - U_L) \quad ; \quad u_L = u_\infty \\
 v_b &= v_L + n_y(U_b - U_L) \quad ; \quad v_L = v_\infty \\
 w_b &= w_L + n_z(U_b - U_L) \quad ; \quad w_L = w_\infty
 \end{aligned}$$

To obtain the thermal properties at the boundary, isentropic process between L and b is assumed, and thus

$$\frac{T_b}{\rho_b^{\gamma-1}} = \frac{T_L}{\rho_L^{\gamma-1}} \Rightarrow \rho_b = \left[\frac{T_b}{T_L / \rho_L^{\gamma-1}} \right]^{\frac{1}{\gamma-1}} \quad \text{and} \quad p_b = \frac{1}{\gamma} \rho_b T_b$$

where


$$T_L = \gamma \frac{p_L}{\rho_L}; \quad p_L = p_\infty; \quad \rho_L = \rho_\infty$$

Modified implementation:

$$\begin{aligned}
 \mathfrak{R}^+ &= U_R + \frac{2a_R}{\gamma_R - 1} = U_b + \frac{2a_b}{\gamma_b - 1} \\
 \mathfrak{R}^- &= U_L + \frac{2a_L}{\gamma_L - 1} = U_b - \frac{2a_b}{\gamma_b - 1}
 \end{aligned} \tag{C.1}$$

and

$$U_R = U_c + \nabla U \cdot \Delta \vec{s}; \quad U_L = U_g = U_\infty; \quad (\alpha_s)_L = (\alpha_s)_g = (\alpha_s)_\infty; \quad R_L = R_\infty \tag{C.2}$$

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where α_i is the mass fraction of i -th species and R is the mixture gas constant. Subscript ∞ denotes the freestream condition. Hence, the condition at the boundary can be obtained as:

$$U_b = \frac{1}{2}(\mathfrak{R}^+ + \mathfrak{R}^-); \quad a_b = \frac{\gamma_b - 1}{4}(\mathfrak{R}^+ - \mathfrak{R}^-) \quad (\text{C.3})$$

If $U_b + U_m \geq 0$ where U_m is the contravariant velocity of the moving boundary, then the information is traveling from the right-hand-side. Hence,

$$\begin{aligned} u_b &= u_R + n_x(U_b - U_R) \\ v_b &= v_R + n_y(U_b - U_R) \\ w_b &= w_R + n_z(U_b - U_R) \\ (\alpha_s)_b &= (\alpha_s)_R = (\alpha_s)_c \quad ; \quad R_b = R_R = f((\alpha_s)_R) \end{aligned} \quad (\text{C.4})$$

Once the speed of sound and the mixture gas constant at the boundary are obtained, an iterative procedure can be used to determine the temperature and the ratio of specific heats at the boundary based on the following correlations.

$$a_b = \sqrt{\frac{\gamma_b R_b T_b}{\gamma_{\text{ref}}}}; \quad \gamma_b = \frac{(C_p)_b}{(C_p)_b - R_b} = \frac{(C_p/R)_b}{(C_p/R)_b - 1} \quad (\text{C.5})$$


$$\left(\frac{C_p}{R}\right)_b = \left(\frac{C_p^o}{R_u}\right)_b = \left(\sum_{s=1}^{NS} n_s \frac{(C_p^o)_s}{R_u}\right)_b; \quad n_s = \frac{\alpha_s/M_s}{\sum_{s=1}^{NS} (\alpha_s/M_s)} \quad (\text{C.6})$$

$$(C_p^o)_s/R_u = (a_1 \bar{T}^{-2} + a_2 \bar{T}^{-1} + a_3 + a_4 \bar{T} + a_5 \bar{T}^2 + a_6 \bar{T}^3 + a_7 \bar{T}^4)_s \quad (\text{C.7})$$

With the isentropic assumption between the upwind cell and the boundary, the mixture density and pressure at the boundary can be calculated based on the temperature (T_c) and mixture density (ρ_c) of the upwind cell as:

$$\rho_b = \left[\frac{T_b}{(T_c/\rho_c^{\gamma_b-1})} \right]^{\frac{1}{\gamma_b-1}}; \quad \text{and} \quad p_b = \frac{1}{\gamma_{\text{ref}}} \rho_b R_b T_b \quad (\text{C.8})$$

Total energy at the boundary is then calculated from temperature, species mass fraction, and velocity components at the boundary based on the caloric equation of state.


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If $U_b + U_m < 0$, then the information is traveling from the left-hand-side. Hence,

$$\begin{aligned}
u_b &= u_L + n_x(U_b - U_L) \quad ; \quad u_L = u_\infty \\
v_b &= v_L + n_y(U_b - U_L) \quad ; \quad v_L = v_\infty \\
w_b &= w_L + n_z(U_b - U_L) \quad ; \quad w_L = w_\infty \\
(\alpha_s)_b &= (\alpha_s)_L = (\alpha_s)_\infty \quad ; \quad R_b = R_R = R_\infty
\end{aligned}
\tag{C.9}$$

The procedure stated above used to solve Equation (C.5) through (C.7) can be used to obtain the thermal properties at the boundary. Finally, the total enthalpy at the boundary can be calculated as:

$$E_b = \int_0^{T_b} (C_p - R)_b dT + \frac{1}{2}(u_b^2 + v_b^2 + w_b^2) \quad \text{and} \quad E_g = E_\infty
\tag{C.10}$$

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Appendix D. Numerical Treatment of Viscous Wall Boundary Conditions

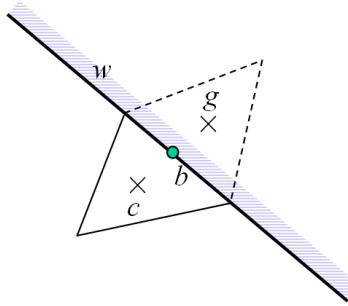


Figure D-1. Orientation of a Wall Boundary Face

Based on the notations used in Figure D-1, the boundary conditions for a solid wall boundary can be summarized as:

$$\begin{aligned}
 u_b &= u_w ; \quad v_b = v_w ; \quad w_b = w_w \\
 u_g &= 2u_b - u_c ; \quad v_g = 2v_b - v_c ; \quad w_g = 2w_b - w_c \\
 \frac{\partial p}{\partial n} &= 0 \Rightarrow \quad p_b = p_c + \nabla p \cdot \Delta \vec{s} ; \quad p_g = 2p_b - p_c
 \end{aligned}$$

Current formulation:

- 1) adiabatic wall:


$$\frac{\partial T}{\partial n} = 0 \Rightarrow T_b = T_c ; T_g = T_c$$

$$\rho_b = \gamma_{\text{ref}} \frac{p_b}{T_b} ; \quad \rho_g = \gamma_{\text{ref}} \frac{p_g}{T_g}$$

- 2) isothermal wall:

$$T_b = T_w \Rightarrow \rho_b = \gamma_{\text{ref}} \frac{p_b}{T_b}$$

$$\rho_g = 2\rho_b - \rho_c$$

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Modified implementation:

$$\frac{\partial \alpha_s}{\partial n} = 0 \Rightarrow (\alpha_s)_b = (\alpha_s)_c; \quad (\alpha_s)_g = (\alpha_s)_c$$

1) adiabatic wall:

$$\frac{\partial T}{\partial n} = 0 \quad \triangleright \quad T_b = T_c; \quad T_g = T_c$$

$$\triangleright \quad r_b = g_{\text{ref}} \frac{p_b}{T_b}; \quad e_b = \int_0^{T_b} C_v dT$$

$$r_g = g_{\text{ref}} \frac{p_g}{T_g}; \quad e_g = \int_0^{T_g} C_v dT$$

$$\text{and} \quad E_b = e_b + \frac{1}{2}(u_b^2 + v_b^2 + w_b^2); \quad E_g = e_g + \frac{1}{2}(u_g^2 + v_g^2 + w_g^2)$$

2) isothermal wall:

$$T_b = T_w \Rightarrow \quad E_b = \int_0^{T_b} C_v dT + \frac{1}{2}(u_b^2 + v_b^2 + w_b^2) \quad \text{and} \quad \rho_b = \gamma_{\text{ref}} \frac{p_b}{T_b}$$

$$\rho_g = 2\rho_b - \rho_c \Rightarrow \quad T_g = \gamma_{\text{ref}} \frac{p_g}{\rho_g} \quad \text{and} \quad E_g = \int_0^{T_g} C_v dT + \frac{1}{2}(u_g^2 + v_g^2 + w_g^2)$$



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Appendix E. Description of USM3D Input File

USM3D (v6.0) - Sample Input File

```

Mach      alpha      beta      ReUe,mil  Tinf,dR    itwall    Tw/Tinf  ipwall
0.84000   3.06000    0.00000  11.7     460.00000  0         -1.0     0
sref      cref        bref      xmc       ymc        zmc
0.52550   0.66700    1.00000  0.00000  0.00000    0.00000
ioverset  impl       cfl1      iramp     cfl2       cflmin    GS_tol   crelax
0         1         -150.000  50       150.       5.0       -20      1.00
itimeacc  delta_t     ntstep    res_step  imvgrd     isolavg    timebgn
-2        0.3       500      -3.0     1          0         1500.0
irest     mstage     iresmth   dqmax    p_break    pmin      limiter
0         3         1        0.5     0.050     0.001     0.
nupdate   nwrest     nwflo     nwflobgn  iptqn      idiagnos   nodeypl
50        75        100      1500    2          0         0
iorder    lapl-avg   high-bc   ifds      ivisc      itrip     ev_lim
2         1         1        1        3          0         0.0
ncyc      nengines   nsinkbc   nrotor    compF&M    p_bc1002  cldes
10        1         1        1        0          0.0       0.0
jet1      fuel       gammaj    pjet      p0jet     Rratio    T0jet
103      0.02000   1.40000  0.71430  1.42857   0.77400   3.17390
jet1      vec(1)     vec(2)    vec(3)    engsim    nstation  idirec
103      1.00000   0.00000  0.00000  0         10        1
jet1      fuel       gammaj    pjet      p0jet     Rratio    T0jet
102      0.02000   1.40000  0.71430  1.42857   0.77400   3.17390
jet1      vec(1)     vec(2)    vec(3)    engsim    nstation  idirec
102      1.00000   0.00000  0.00000  1         10        1
jet1      inner_R    outer_R   cen_X     cen_Y     cen_Z
102      1.0114    1.39846  23.646   8.713    -3.322
(r-inner_R)/(outer_R-inner_R)
0.168,0.350,0.500,0.600,0.700,0.800,0.900,0.950,0.975,1.00
p0jet
1.07143 1.07143 1.07143 1.07143 1.07143 1.07143 1.07143 1.07143 1.07143 1.07143
T0jet
1.32610 1.32610 1.32610 1.32610 1.32610 1.32610 1.32610 1.32610 1.32610 1.32610
V_circular/Vmag
0.0168 0.035 0.050 0.060 0.070 0.080 0.090 0.095 0.0975 0.1
V_radial/Vmag
0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
sinkid   outer_R   cen-X     cen-Y     cen-Z     massflx   omega
111     1.0      0.0      0.0      0.0      3.0      -0.5
rotid    inner_R   outer_R   cen-X     cen-Y     cen-Z
502     0.00000  24.0000  0.0      0.0      0.0
Advratio thrst_c   torq_c    irotat    rotsim
0.20    0.00861  0.00     1         0
Xrcg    Yrcg     Zrcg     reflen    iroll     ipitch    iyaw
0.0     0.0     0.0     1.0      0         1         0
ang_mean ang_ampl  red_freq  ideformg  imvMOMCEN
0.00    2.41    0.0808  0         0
ikeord   icons     nstagek   t_dtfact  t_intsity  mut/mul   ratiokp   dkemax
1        1        5         1.0      1.e-3     1.0      0.00     0.25
inl      ilhg     iwallf    icompCorr itempCorr  itk       isk       idt_proc
7        -14     0         0         0         2         1         0

```



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```

flkemax <=== THIS IS A TEMPORARY VARIABLE FOR CAPPING MAX f1 in LB MODEL
1.0
$SPECIES
H2O O2 CO CO2 C7H8 H2 O H OH N2
$REACTIONS
13
REACTION:H2O, O2, CO, CO2, C7H8, H2, O, H, OH, N2,
1, 4.4963E9, 1.00, 2.679E4, 0, 2,
0., -3.5, 7., 0., -1., 4., 0., 0., 0., 0.,
0., -1.0, 0., 0., -0.5, 0., 0., 0., 0., 0.,
2, 1.7000E13, 0.00,24070., 0, 0,
0., -1., 0., 0., 0., -1., 0., 0., 2., 0.,
3, 2.1900E13, 0.00, 2590., 0, 0,
1., 0., 0., 0., 0., -1., 0., 1., -1., 0.,
4, 6.0230E12, 0.00, 550., 0, 0,
1., 0., 0., 0., 0., 0., 1., 0., -2., 0.,
5, 1.8000E10, 1.00, 4480., 0, 0,
0., 0., 0., 0., 0., -1., -1., 1., 1., 0.,
6, 1.2200E17, -0.91, 8369., 0, 0,
0., -1., 0., 0., 0., 0., 1., -1., 1., 0.,
7, 4.0000E12, 0.00,10030., 0, 0,
0., 0., -1., 1., 0., 0., 0., 1., -1., 0.,
8, 3.0000E12, 0.00,2.50E4, 0, 0,
0., -1., -1., 1., 0., 0., 1., 0., 0., 0.,
9, 1.0000E16, 0.00, 0.,999, 0,
0., 0., 0., 0., 0., 0., -1., -1., 1., 0.,
10, 2.5500E18, -1.00,59390.,999, 0,
0., 1., 0., 0., 0., 0., -2., 0., 0., 0.,
11, 5.0000E15, 0.00, 0.,999, 0,
0., 0., 0., 0., 0., 1., 0., -2., 0., 0.,
12, 8.4000E21, -2.00, 0.,999, 0,
1., 0., 0., 0., 0., 0., 0., -1., -1., 0.,
13, 6.0000E13, 0.00, 0.,999, 0,
0., 0., -1., 1., 0., 0., -1., 0., 0., 0.,

```

```

=====
c LINE 1
c Title - free form upto 80 characters
=====
c LINE 2
c xmach - freestream Mach number
c for xmach < 0, velocity will be initialized by
c a fixed mach value of 0.4. Some usefulness for supersonic cases,
c however *not* recommended.
c alpha - angle of attack, deg. (in X-Z plane)
c beta - side-slip angle, deg. (in X-Y plane)
c reue - freestream Reynolds number per unit length (millions)
c tinf - freestream temperature (degrees Rankine)
c itwall - wall temperature boundary condition flag
c = 0 adiabatic wall temperature
c = 1 specified wall temperature
c twtinf - wall temperature (temperature at wall divided by temperature
c of freestream)
c if twtinf<=0, twtinf taken as freestream stagnation temperature)

```



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```
c      ipwall - type of extrapolation of pressure to wall
c              = 0 zeroth order
c              = 1 first order (linear extrapolation)
c
c-----
c LINE 2
c      igmodel - flag to specify gas model
c              = 0 Air (calorically perfect)
c              = 1 Any gas with specified sutherland const and gamma
c                (calorically perfect)
c              = 2,-2 Any gas with specified sutherland const, gamma, and
c                  gas name (to set temperature variation of gamma)
c              = 3,-3 Two-gas model with specified gamma, sutherland const,
c                  stagnation enthalpies, and gas names
c              -2 or -3 is Recommended
c      gammal,gamma2 - specific heat ratios (gamma)
c      htot1,htot2 - total enthalpies (non-dimensional)
c      numspec - total number of species constituting 1- or 2-gas system
c      NOTE      : For igmodel values of 2 or 3, user must have "thermo.inp"
c                  file of McBride and Gordon.
c                  : For igmodel=2 or 3, you can set gammal<=0; code will
c                  calculate the value internally based on freestream temp.
c                  : For igmodel=3, you can set Htot1<= 0; code will calculate
c                  the value internally.
c                  : For igmodel=3, and exit BC -102, you can set Htot2<= 0;
c                  code will calculate the value internally.
c
c-----
c LINE 3
c      gasname - Name of a gas (must be part of McBride-Gordon table)
c      ispec_grp - specie group index, must be 1 or 2 (2-gas model)
c      mole_frac - Mole fraction of the gas in a given specie group
c
c-----
c LINE 5
c      sref - reference area (half-area for half configuration)
c      cref - reference length
c      bref - reference span
c      xmc - moment center in x-direction
c      ymc - moment center in y-direction
c      zmc - moment center in z-direction
c
c-----
c LINE 6
c      ioverset - overset grid flag
c              = 0 single grid
c              = 1 overset grid
c      impl - implicit time stepping flag
c              = 0 explicit Runge-Kutta time stepping
c              = 1 implicit Gauss-Seidel time stepping
c              = 1 UPDATQ, timestep scaling; UPDATQ enforces positive-
c                  definite updates for density & internal energy
c              = 10 UPDATQ, timestep scaling off
c              = 2 UPDATQ1, timestep scaling; UPDATQ1 *does not*
c                  change solver-provided solution updates
c              = 20 UPDATQ1, timestep scaling off
```



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```
c          = 3 UPDATQ2, timestep scaling
c          = 30 UPDATQ2, timestep scaling off
c          code will internally reset impl to 1 after raising
c          appropriate flags.
c      cfl1  - time step or initial clf number
c          < 0 local time stepping or ramping
c      iramp - number of cycles for ramping cfl number
c      cfl2  - final value of cfl number for ramping
c      cflmin - minimum allowable CFL for variable time step strategy
c      GS_tol = Tolerance criterion for automatic termination of Gauss-Seidel
c          iteration process termination for Flow and S-A equations
c          recommended value (1-dq_prev/dq_new) is 0.001-0.005.
c          = Negative value will be interpreted as G-S stages
c          by the code for solving linear problem for mean flow.
c          Minimum threshold value for stages is set to 5.
c      crelax = Under/over-relaxation coefficient for Newton's scheme.
c          = 0.7 as recommended by Dr. Paul Pao.
c          Without this relaxation, Newton's scheme produced jagged
c          hysteresis of Lift and moment coefficients for
c          NACA 0012 viscous pitching case.
c
c          *CAUTION* itimeacc=0, 1 or 2 options also will use relaxation
c          coefficient. For itimeacc=2, relaxation is not typically
c          needed. Therefore it is important to set it to 1.0 when
c          not using Newton's scheme (itimeacc=-2).
c-----
c LINE 7
c      itimeacc = 0 Not time accurate; assumes steady state final solution
c          = 1 Time-accurate solution with subiterations using
c          Crank-Nicholson
c          = 2 Time-accurate solution with subiterations using
c          3-point backward differencing and pseudo-time
c          =-2 Time-accurate solution with subiterations using
c          3-point backward differencing without pseudo-time (Newton)
c      delta_t - time step increment (nondimensional)
c          HOW DOES ONE DETERMINE VALUE FOR TIMESTEP?
c          -> Think of it as how many timesteps one needs for a fluid
c          particle to travel some characteristic length, Lchar,
c          e.g. wing chord, at freestream velocity. A rule of thumb
c          from Jim Forsythe, Cobalt Solutions, is N=50 steps.
c          Scott Morton of the Air Force Academy suggests between
c          100 and 1000 steps.
c          -> For USM3D nondimensionalization, the relationship for
c          timestep and number of steps, N, to traverse Lchar:
c          delta_t = Lchar/xmach/N
c      ntstep  - number of timestep increments
c          (Note that total "iterations" will be approx. ntstep*ncyc)
c      res_step - level of subiteration convergence before taking next step
c          Typical value might be -2 or -3.
c      imvgrd  - invokes prescribed grid motion
c          (additional input required, see LINE 5a below)
c      isolavg - solution averaging flag
c          = 0, turn-off solution averaging (for steady-state, it will
c          be turned off by the code)
c          = 1, perform time averaging for mean flow solution quantities
```



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```
c          (extra memory equivalent to 5*nnode). Also, mean values
c          of aerodynamic quantities will be printed.
c          = 2, In addition to 1 above, perform solution averaging for
c          turbulent-stress-related quantities (extra memory
c          equivalent to 11*nodes)
c          timebgn - beginning timestep for initiating time-averaging of solution
c          (based on the "ntstep" timestep numbering, not "ncyc")
c
c NOTES: 1) "ncyc" becomes the number of subiterations+1 used to converge
c          solution to Q_(n+1)
c          2) Need to monitor hist.subit for subiteration convergence
c
c-----
c LINE 8
c   irect = 0 no restart
c         = 1 restart
c   mstage - number of Runge-Kutta stages (for explicit scheme)
c           For implicit scheme mstage < 0 specifies interval at which
c           all the cells are reset as second-order cells
c   iresmth - implicit residual smoothing (for explicit scheme)
c           = 1 smoothing on every m-stage cycle
c           = -1 smoothing only on odd m-stage cycles
c           For implicit scheme iresmth specifies technique to mark
c           first order cells
c           = 0 => do not set cells to first order locally
c           = 1 => use p<=pminimum or rho<=pminimum switch to set
c           first order cells
c           = 2 => use p<=pminimum or rho<=pminimum or pt>=1.2*pt0
c           switch to set first order cells iresmth=2 will
c           only be used for non-engine, non-rotor cases
c   dqmax - maximum allowable (-dp/p, -drho/rho) in solution
c           (used to scale CFL number)
c           = 0.5 suggested
c           = greater than zero --> No Limiter Applied
c   pbrk   = threshold pressure for lowering local CFL toward CFLMIN
c   pminimum= Minimum allowable level of non-dimensional pressure and
c           threshold for setting cells to 1st order
c           <0 also resets 1st-order flagged cells to 2nd-order
c   bcoef  - Limiter coefficient
c           = 0. no limiting
c           = 1. MINMOD limiter
c           = 2. SUPERBEE limiter with variable compression factor
c           = -2. will involve automatic selection of limiter
c
c-----
c LINE 9
c   nupdate - number of iterations between updates of the time step
c           (not used for time accurate computations)
c   nwrest  - number of iterations between updates of the binary
c           restart file
c           - for UNSTEADY runs (itimeacc.NE.0), this is restart file
c           updates are based on the number of "ntstep", not "ncyc"
c   nwflo   - number of iterations between writing of instantaneous
c           NEW flow-file (prj_name.flo.iter#). Typically used for
c           time-accurate runs.
```



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```
c  nwflobgn  - number of iterations beyond which writing of instantaneous
c             NEW flow-file (prj_name.flo.iter#) will be triggered.
c             The parameters nwflo and nwflobgn relate to outer loop
c             time steps (ntstep) for an unsteady flow analysis
c             and to inner loop time steps (ncyc) for steady flow analysis.
c  ipltqn    = 0 suppress output of post analysis of flow field file
c            = 1 write unformatted q-node file for post analysis of flow field
c            = 2 write formatted q-node file for post analysis of flow field
c            = 3 write formatted q-node file for postprocessing by TECPLOT
c            = 4 write binary TECPLOT file (NOT CODED YET)
c            = 5 write unformatted q-node file for postprocessing by FIELDVIEW
c            X  =13 write unformatted q-node file for using Tecplot converter
c            X  =23 write formatted q-node file for using Tecplot converter
c            =15 write unformatted q-node file for using FIELDVIEW converter
c            =25 write formatted q-node file for using FIELDVIEW converter
c            =-25 write solution restart file for using FIELDVIEW converter
c                also write formatted q-node file and do not delete
c            X  =16 write unformatted q-node file for using Enight converter
c            X  =26 write formatted q-node file for using Enight converter
c            X  =  **indicates that this option has not been tested and**
c                **not recommended for use.**
c  idiagnos= 0 no output
c            1 write history of minimum static pressure, maximum
c              Mach number, maximum eddy viscosity in info.diag file.
c            2 write a flow file with 5 auxiliary variables in place of Qs
c              for unsteady flow simulations. These variables are,
c              instantaneous and time-average values of vorticity,
c              eddy viscosity, and local CFL number.
c            3 write info.diag2 file in Tecplot format that contains
c              several variables at cell-centers for the cells associated
c              with user-specified boundary faces. These boundary faces
c              must be supplied in project.trip file. You will need to
c              create a project.trip file for idiagnos != 3 as well, if
c              itrip != 0 (below). NOTE: Diagnostics related to
c              idiagnos = 3 is available only for ivisc > 0.
c            4 write info.probe.N file in Tecplot format that contains
c              history of Qs for each probe specified in project.probe
c              file. N will be substituted by the probe number.
c            5 write "Sol.Volume.USM3D" file in PLOT3D format that contains
c              Qs at desired locations in the grid as read from the file
c              "Grid.Volume.TEACC" in a pre-processing step. In addition,
c              "Sol.Exit.TEACC" file will be read at appropriate time to
c              derive exit pressures for appropriate locations on the
c              boundary. These locations are written out in the file
c              "Grid.Exit.USM3D".
c  nodeypl= # Boundary node number where output of u+/y+ is desired
c            0 no output
c
c-----
c LINE 10
c  iorder    = order of flux computation
c            = <0 (INTEGER only) Automatic selection of order based on
c              prescribed magnitude of mean-flow residual error drop
c            = 0 Automatic selection of order based on residual error drop
c              by one order
```




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```
c          = 1  first order
c          = 2  Taylor series with full gradient computation
c  laplavg = 0  Inverse-distance averaging to all nodes (Vers. 1.0)
c          = 1  Pseudo-Laplacian averaging to all nodes
c          = -1 (Ps. Lapl. on interior, Inv. Dist. on boundary nodes)
c  ihibc   = 0  First-order accurate boundary conditions (Vers. 1.0)
c          = 1  Second-order accurate boundary conditions
c  ifds    -  spatial differencing parameter for Euler fluxes
c          = 0  flux-vector splitting
c          = 1  flux-difference splitting (Roe scheme) (recommended)
c          = 2  AUSM+ (need to evaluate for USM3D (as of 06/17/04).
c          = 3  HLLC (need to evaluate, only for stationary cases
c              as of 07/12/05)
c  ivisc   -  viscous/inviscid interaction flag
c          = 0  inviscid
c          = 1  laminar (not active in version 2.0)
c          = 2  Spalart-Almaras, full viscous
c          = -2 Spalart-Almaras, full viscous with DES
c          = 3  Spalart-Almaras with wall function
c          = -3 Spalart-Almaras with wall function with DES
c          = 6  K-Epsilon turbulence model
c          = -6 K-Epsilon turbulence model with DES
c          = -60 K-Epsilon turbulence model with Multiscale capability
c          = 7  K-Epsilon turbulence model, Carlson's formulation
c          = 8  SST turbulence model
c          = -8 SST turbulence model with DES capability
c          = -80 SST turbulence model with Multiscale capability
c  itrip   -  flag to activate flow tripping
c          = 0  no tripping
c          = 1  activates tripping (useful mostly for k-e turbulence model
c              when used for low Reynolds number flows)
c          = -1 enforces laminar flow region (useful mostly for SA and
c              SST model when a certain flow region has to be forced
c              to a laminar flow state. These two models generally
c              provide a fully turbulent flow on the body).
c              NOTE: for itrip value other than 0, user will need to
c                  (1) define trip patches in the existing grid
c                      using PREDISC program (contact: Richard Campbell,
c                      LaRC)
c                  (2) create a file project.trip and list all the
c                      trip patches and appropriate trip values.
c                      Refer to the format of project.trip file on
c                      the USM3D website. You will need to create
c                      project.trip file for itrip = 0 as well, if
c                      idiagnos = 3 (above).
c  ev_lim  =  Eigenvalue limiter value
c
c  NOTE: iorder automatic switch should be used only for steady-state cases.
c        If you want to force first order computations based on
c        previous second-order solution upon restart, you must
c        set iorder = 1. Negative iorder value will not let you
c        restart the solution in first order mode.
```

c LINE 11



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```
c fuel = fuel fraction - in % of total exhaust mass flow
c gammaj = ratio of specific heats for (hot) jet
c pjet = static nozzle pressure (usually set to p_infinity)
c p0jet = stagnation pressure of jet
c Rratio = spec. gas constant of air/spec. gas constant of jet
c T0jet = stagnation temperature of jet
c vec(i) = directional cosines of exhaust jet (i=1,2,3 for x,y,z)
c engsim = 0 uniform exhaust properties such as p0jet,t0jet
c = 1 radially varying exhaust properties
c will need radial distribution of total pressure,
c total temperature, tangential and radial velocities.
c nstation = number of radial locations at which exhaust properties
c specified (only useful for engsim=1). LIMIT: nstation <=20.
c idirec = direction of tangential velocity (only useful for engsim=1)
c = 1 clockwise swirl on engine exhaust looking downstream
c = -1 counter-clockwise swirl on engine exhaust looking downstream
c-----
c NPR = nozzle pressure ratio, p0jet/pjet
c TTR = total temperature ratio, T0jet/T0inf
c RMACHJ = exit mach number of jet
c
c-----
c LINE 11b
c sinkid = sink bc identification
c sink 1(BC 111), sink 2(BC 211), sink 3(BC 311)...
c #of sink bcs specified earlier in the input as nsinkbc,
c nsinkbc <= 4
c outer_R = outer radius of sink
c cen-X
c cen-Y
c cen-Z = sink BC's center coordinates
c massflx = mass flow rate through the sink (unit ???)
c -> nondimensional_massflx = dimensional{mdot/(rho*ainf)}
c omega = ratio of fan-tip velocity to freestream velocity
c positive for clockwise looking downstream
c negative for counter-clockwise looking downstream
c
c-----
c LINE 11c
c rotid = rotor identification
c rotor 1 - BC 501,502
c rotor 2 - BC 601,602
c rotor 3 - BC 701,702
c rotor 4 - BC 801,802
c inner_R = inner radius of the rotor
c outer_R = outer radius of the rotor
c cen-X,cen-Y,cen-Z = rotor center coordinates
c Advratio = advance ratio (free stream velocity/rotor tip speed)
c thrst_c = thrust coefficient of rotor
c torq_c = torque coefficient of rotor
c irotat = direction of rotation (viewing from front/top)
c = 1 clockwise rotation
c = -1 counterclockwise rotation
c rotsim = 0 rotor bc with uniform jump in pressure and/or swirl
c = 1 rotor bc with pressure and/or swirl jump as f(r)
```

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```

-----
c LINE 12a
c..CAUTION: These two lines of input read/needed ONLY IF imvgrd != 0 in LINE 4
c..CAUTION: Current implementation set up to allow only 1 DOF for rotation.
c
c   xrcg, yrcg, zrcg - origin of the rotation axis
c   refln           - reference length, used for calculating reduced
c                   frequency, based on grid coordinates
c   iroll           - grid rotation about x-axis (rotation axis || x-axis)
c                   = 1 for activating rolling motion
c                   = 0 for NOT activating rolling motion
c   ipitch          - grid rotation about y-axis (rotation axis || y-axis)
c                   = 1 for activating pitching motion
c                   = 0 for NOT activating pitching motion
c   iyaw            - grid rotation about z-axis (rotation axis || z-axis)
c                   = 1 for activating yawing motion
c                   = 0 for NOT activating yawing motion
c   angmean         - mean angle of rotation (in degrees)
c   angampl         - amplitude of rotation (in degrees)
c   rfreq           - reduced frequency of oscillations (rfreq=k/Lchar) where
c                   k=2*pi*f*Lchar/(2*V_inf), where f is frequency, Lchar is
c                   characteristic length, where all quantities are in
c                   dimensional form
c                   - The number of "steps" required to cycle through one
c                   2*pi period of motion can be computed via.
c                   Nperiod = pi*Lchar/(k*xmach*delta_t)
c   ideformg        - grid deformation flag, important only for itimeacc=2.
c                   = 0 for solid-body rotation of grid,
c                   value of 0 will switch off Geometric Conservation Law.
c                   = 1 for grid deformation to accommodate body motion,
c   imvMOMCEN       - 0 do not rotate moment reference center with the grid
c                   = 1 rotate moment reference center with the grid
c                   (recommended)
c
cNOTE
c..angle for pitch (positive angle for nose up)
c..angle for roll (positive angle for right wing up)
c..angle psi for   (positive angle for left turn, wind blowing in pilot's
c..left ear)
-----
NOTE: VGRID generated proj.cogsg file will now be protected. (Aug 31, 2005)
-----
c LINE 13a
c..CAUTION: These three lines of input read/needed ONLY IF ivisc = 6,7,or,8
c
c   ikeord          - spatial order of accuracy for 2-equation
c                   turbulence models
c                   = 1, first order
c                   = 2, second order
c                   Recommended value is 1
c   icons           - Flag to activate either incompressible or compressible
c                   formulations of for 2-equation turbulence models
c                   = -1, incompressible
c                   = 1, compressible, conservative formulation

```



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```
c
c           Recommended value is 1
c           nstagek - Gauss-seidel subiterations for the implicit solution
c                   of 2-equation turbulence models
c           Recommended value is 10
c           t_dtfact - parameter to decrease/increase CFL number for the
c                   solution of 2-equation turbulence models
c                   > 1.0 decreases CFL number
c                   < 1.0 increases CFL number
c           Recommended value is 1.0
c           t_intsity - freestream turbulence intensity
c                   Recommended value is 1.0e-3
c           mut/mul - ratio of freestream turbulence viscosity to the
c                   freestream laminar viscosity
c                   *NOTE*: You can specify either turbulence intensity
c                   (t_intsity) < 0 or ratio of turbulence-to-laminar
c                   viscosity (mut/mul) < 0 to activate USM3D's default
c                   values of freestream turbulence intensity
c                   [=sqrt(9.e-9)] and mut/mul[=0.009]
c           ratiokp - Upper limit on turbulence kinetic energy in relation
c                   to static pressure
c                   Recommended value: 0.0 for first attempt at solution
c                   If convergence problems are encountered specify
c                   a value in the range of 0.05-0.1
c           dkemax - Maximum allowed update of turbulence model variables
c                   at any given time step (=Delta(var)/var)
c                   Recommended value: 0.25
c
c -----
c LINE 13b
c           inl - Integer to activate different formulations of two
c                   equation turbulence models
c                   0 = Basic turbulence stress model, assumes that
c                   stresses are linearly related to the strain
c                   1 = Nonlinear model of Shih, Zhu, and Lumley
c                   Ref. AIAA-95-2246
c                   7 = Nonlinear model of Girimaji
c                   Ref. NASA CR-198243, 1995
c                   *NOTE*: Currently, only k-eps model has provision to
c                   activate different formulations. For SST model, only
c                   one value (inl=0) is allowed and user input will be
c                   overridden if an inconsistent value is specified for
c                   this model
c           ilhg - Near-wall modification of k-eps turbulence model
c                   -14 = Formulation proposed by Launder and Sharma
c                   -3 = Formulation proposed by Launder and Sharma with
c                   wall function
c                   +3 = No near-wall modification of k-eps turbulence
c                   model but use wall function
c                   Recommended value: -14
c           iwallf - Flag to specify wall function grid
c                   0 = grid suitable for integration all the way to wall
c                   1 = wall function grid
c                   Recommended value: 0
c           icompCorr - Formulations for correction to the turbulence models
c                   related to compressibility at high speeds
c                   0 = no correction applied
```

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```

c          1 = Sarkar's formulation, Ref: J. of Fluid Mechanics,
c                                     Vol. 227, 1991
c          2 = Zeman's formulation, Ref: Physics of Fluids,
c                                     Vol. 2, 1990
c          5 = Wilcox's formulation, Ref: AIAA Paper 92-0439
c          Recommended value: 1
c      itempCorr - Flag to adjust (for linear k-e model only) eddy
c                viscosity for high-temperature flowfields,
c                for example, hot jets.
c                0 = no adjustment made
c                1 = temperature correction model of Hamid
c                   Ref: J. of Fluids Engg., Vol. 126, No. 4, 2004.
c      itk      - Strategies for applying wall boundary condition for
c                the turbulence dissipation variable of k-e model
c                0 = isotropic component of dissipation set to zero
c                   (Launder and Sharma model)
c                1 = zero gradient of dissipation rate at the wall
c                   (Lam and Bremhorst model)
c                2 = dissipation proportional to turbulence kinetic
c                   energy gradient at the wall
c                Recommended value: 2
c      isk      - Flag to apply correction from turbulence kinetic
c                energy equation to the mean-flow energy equation
c                0 = no modification
c                1 = apply corrections
c                Recommended value: 0
c      idt_proc - Flag to activate a specific procedure to compute local
c                time-steps for steady-state solutions
c                0 = use face-based subroutine (UCTIME_MOD)
c                1 = use node-based subroutine (UCTIME_KE)
c                For SA and SST models, idt_proc is reset to 0
c                internally.
c                NOTE: This input variable is introduced in light of
c                the observed sensitivity of a CEV solution (Run 314)
c                to the differences in the procedure used to compute
c                local time steps. This option may be eventually
c                dropped from the export version 6.0.
c-----
c LINE 13c
c      flkemax - Maximum allowed value for function f1 in dissipation
c                rate equation for Lam Bremhorst model (itk=1)
c                Recommended value : 1.0
c                for itk = 0 and 2 this input variable is not used.


```

Supplemental Description of Input for Real Gas and Chemical Reactions

\$SPECIES: flag to activate real-gas model for single or multiple chemical species

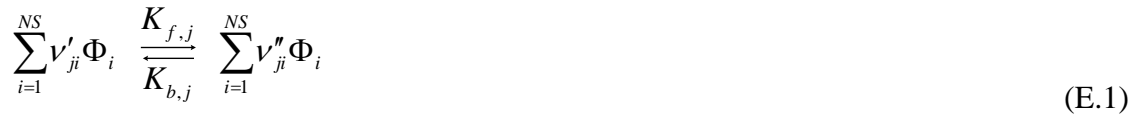
The above line is followed by a list of species names involved in this test case. The name of each species can be either separated by blank space(s) or comma. An example is shown below:
H₂O O₂ CO CO₂ C₇H₈ H₂ O H OH N₂

\$REACTIONS: flag to activate chemical reactions

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The above line is followed by the number of chemical reaction steps (NR). If NR is negative, then equilibrium chemistry will be used. If the specified value is greater than 0, then the finite-rate chemistry will be used where the value indicates the number of reaction steps. The format of finite-rate chemistry model is listed below. As shown in Equation (E.1), a general system of chemical reactions can be written in terms of its stoichiometric coefficients:

(ν'_{ij} and ν''_{ij}) and the i -th chemical species (Φ'_{ij} and Φ''_{ij}) for the j -th reaction:



The source term of i -th species ($\dot{\omega}_i$), due to chemical reaction, can be evaluated as:

$$\dot{\omega}_i = M_i \sum_{j=1}^{nr} \nu_{ji} \left\{ K_{f,j} \prod_{l=1}^{ns} \left(\frac{\rho \alpha_l}{M_l} \right)^{r'_{jl}} - K_{b,j} \prod_{l=1}^{ns} \left(\frac{\rho \alpha_l}{M_l} \right)^{r''_{jl}} \right\} \quad (\text{E.2})$$

where M_i is the molecular weight of species “ i ”, nr is the total number of reactions, ν_{ji} is the stoichiometric coefficient, $K_{f,j}$ and $K_{b,j}$ are the forward and backward reaction rates of the j^{th} reaction, and ns is the total number of species. r'_{ij} and r''_{ij} are the power dependence of the reactant and product, respectively. The reaction rate, in general, is formulated in the empirical Arrhenius form as:

$$K_{f,j} = A_j T^{B_j} e^{-E_{a,j}/R_u T} \quad (\text{E.3})$$

where A_j , B_j , $E_{a,j}$ are empirical constants for j -th reaction. The input format is shown in the following table, where E/R is $E_{a,j}/R_u$, STCOEF is ν_{ji} , and STCOEG is r_{ji} .



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Format (2 or 3 lines*NR)	REACTION: Species names, $i = 1 \rightarrow ns$ (only 1 line as a title) j , A, B, E/R, ITHIRD, IGLOB, (STOCEF(i, j), $i = 1 \rightarrow ns$), (STOCEG(i, j), $i = 1 \rightarrow ns$)* * needed if IGLOB = 2
Definition	j reaction step counter
	A reaction rate leading constant
	B reaction rate temperature exponent
	E/R reaction rate activation energy constant
	ITHIRD third-body reaction indicator = 0: deactivated = n : for using the n -th species as third-body = 999: for global (every species) third-body
	IGLOB global reaction model indicator = 0: elementary reactions with the rate of backward reaction is calculated from equilibrium constant and forward reaction rate = 1: one-way reaction (either forward or backward reaction controlled by the sign of STCOEF); need only one input line of STCOEF = 2: one-way reaction with power dependency; need input line for STCOEF and STCOEG
	STCOEF stoichiometric coefficients of elementary reactions (negative signs apply to reactants and positive signs are for the products)
STCOEG power dependency coefficients (negative signs apply to reactants and positive signs are for the products)	

For a sample reaction model:

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```
REACTION:H2O, O2, CO, CO2, C7H8, H2, O, H, OH, N2,
  1, 4.4963E9, 1.00, 2.679E4, 0, 2,
    0., -3.5, 7., 0., -1., 4., 0., 0., 0., 0.,
    0., -1.0, 0., 0., -0.5, 0., 0., 0., 0., 0.,
  2, 1.7000E13, 0.00,24070., 0, 0,
```




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0., -1., 0., 0., 0., -1., 0., 0., 2., 0.,
3, 2.1900E13, 0.00, 2590., 0, 0,
1., 0., 0., 0., 0., -1., 0., 1., -1., 0.,
4, 6.0230E12, 0.00, 550., 0, 0,
1., 0., 0., 0., 0., 0., 1., 0., -2., 0.,
5, 1.8000E10, 1.00, 4480., 0, 0,
0., 0., 0., 0., 0., -1., -1., 1., 1., 0.,
6, 1.2200E17, -0.91, 8369., 0, 0,
0., -1., 0., 0., 0., 0., 1., -1., 1., 0.,
7, 4.0000E12, 0.00, 10030., 0, 0,
0., 0., -1., 1., 0., 0., 0., 1., -1., 0.,
8, 3.0000E12, 0.00, 2.50E4, 0, 0,
0., -1., -1., 1., 0., 0., 1., 0., 0., 0.,
9, 1.0000E16, 0.00, 0., 999, 0,
0., 0., 0., 0., 0., 0., -1., -1., 1., 0.,
10, 2.5500E18, -1.00, 59390., 999, 0,
0., 1., 0., 0., 0., 0., -2., 0., 0., 0.,
11, 5.0000E15, 0.00, 0., 999, 0,
0., 0., 0., 0., 0., 1., 0., -2., 0., 0.,
12, 8.4000E21, -2.00, 0., 999, 0,
1., 0., 0., 0., 0., 0., 0., -1., -1., 0.,
13, 6.0000E13, 0.00, 0., 999, 0,
0., 0., -1., 1., 0., 0., -1., 0., 0., 0.,

```

Reaction Step	<i>A</i>	<i>B</i>	E_a/R_u	Power Dependencies (r_{ij})
$C_7H_8 + 3.5O_2 \rightarrow 7CO + 4H_2$	4.4963E9	1	2.679E4	$[C_7H_8]^{0.5} [O_2]^1$
$H_2 + O_2 \leftrightarrow OH + OH$	1.7E13	0	2.407E4	---
$OH + H_2 \leftrightarrow H_2O + H$	2.19E13	0	2.59E3	---
$OH + OH \leftrightarrow O + H_2O$	6.023E12	0	5.5E2	---
$O + H_2 \leftrightarrow H + OH$	1.8E10	1.0	4.48E3	---
$H + O_2 \leftrightarrow O + OH$	1.22E17	-0.91	8.369E3	---
$H + O + M \leftrightarrow OH + M$	1.0E16	0	0	---
$O + O + M \leftrightarrow O_2 + M$	2.55E18	-1.0	5.939E4	---
$H + H + M \leftrightarrow H_2 + M$	5.0E15	0	0	---

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$H + OH + M \leftrightarrow H_2O + M$	8.4E21	-2.0	0	---
$CO + OH \leftrightarrow H + CO_2$	4.0E12	0	4.03E3	---
$CO + O_2 \leftrightarrow CO_2 + O$	3.0E12	0	2.5E4	---
$CO + O + M \leftrightarrow CO_2 + M$	6.0E13	0	0	---

Note: M represents the third body, which includes all species in the above reaction model. If the power dependency is not specified, then the stoichiometric coefficient will be used.

REPORT DOCUMENTATION PAGE

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14. ABSTRACT The USM3D Navier-Stokes flow solver contributed heavily to the NASA Constellation Project (CxP) as a highly productive computational tool for generating the aerodynamic databases for the Ares I and V launch vehicles and Orion launch abort vehicle (LAV). USM3D is currently limited to ideal-gas flows, which are not adequate for modeling the chemistry or temperature effects of hot-gas jet flows. This task was initiated to create an efficient implementation of multi-species gas and equilibrium chemistry into the USM3D code to improve its predictive capabilities for hot jet impingement effects. The goal of this NASA Engineering and Safety Center (NESC) assessment was to implement and validate a simulation capability to handle real-gas effects in the USM3D code. This document contains the outcome of the NESC assessment.					
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