

Three-Dimensional Nonequilibrium Boundary Layer Stability & Transition Analysis For Martian Entry

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In this work, we apply the boundary layer stability code LASTRAC, modified to include chemical and thermal nonequilibrium capabilities, to a simulated test case based on literature, with three-dimensional effects. LASTRAC provides Parabolized Stability Equations (PSE) as well as Linear Stability Theory (LST) to predict the stability of a boundary layer and transition with semiempirical e^N methods. Tests of the Mars Science Laboratory (MSL) indicated a range of laminar to transitional flow conditions. In order to reduce the weight of Thermal Protection Systems (TPS), reliable prediction of transition and an understanding of the environmental factors that contribute to transition are necessary. This work is a step towards addressing this need, including the effects of thermochemical nonequilibrium but neglecting radiation, ablation, and ionization effects. Our results indicate that an oblique first mode produces maximum N-Factors on the symmetry plane, however with N-Factors too small to explain transition. Although we are able to show nonequilibrium three-dimensional PSE results in CO_2 , further study with improved mean flow solutions, accounting for some of the uncertainties inherent in this analysis, or evaluation of alternative transition mechanisms is needed to explain transition in the wind tunnel cases examined here.

I. Nomenclature

ρ	= density [kg m ⁻³]
p	= pressure [Pa]
T	= temperature [K]
e	= energy per unit mass [J kg ⁻¹]
h	= enthalpy per unit mass [J kg ⁻¹]
C_s	= mass fraction for species s
k	= thermal conductivity [J m ⁻¹ s ⁻¹ K ⁻¹]
t	= time [s]
f	= frequency [Hz]
ℓ	= boundary layer length scale [m]
x, y, z	= body-fitted coordinates
$\vec{V}$	= velocity vector [m/s]
M_s	= molar mass for species s [g/mol]
α_i	= imaginary component of complex wave number α
β	= spanwise wave number
γ	= ratio of specific heats
λ	= second viscous coefficient [N s m ⁻²]
μ	= viscosity [N s m ⁻²]
ν	= dynamic viscosity [kg s ⁻¹ m ⁻¹]
ϕ	= disturbance vector
τ_s	= vibrational-translational relaxation time [s]

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$\dot{\omega}_s$	= species production rate [$\text{kg m}^{-3} \text{s}^{-1}$]
ω	= streamwise wave number
D_s	= diffusion coefficient of species s with respect to the mixture [$\text{m}^2 \text{s}^{-1}$]
C_p, C_v	= constant pressure and constant volume specific heats [$\text{J mol}^{-1} \text{K}^{-1}$]
$C_{p,s}, C_{v,s}$	= constant pressure and constant volume specific heats for species s [$\text{J mol}^{-1} \text{K}^{-1}$]
$C_{v,V}^s$	= constant volume specific heat for vibrational energy for species s [$\text{J mol}^{-1} \text{K}^{-1}$]
k_B	= Boltzmann's constant [J K^{-1}]
Av	= Avogadro's number [mol^{-1}]
R_u	= universal gas constant [$\text{J mol}^{-1} \text{K}^{-1}$]
Re	= Reynolds number
Re_{cf}	= crossflow Reynolds number
Re_u	= unit Reynolds number [m^{-1}]
Le	= Lewis number
Pr	= Prandtl number
Ec	= Eckert number
M	= Mach number
F	= nondimensionalized frequency
$()_s$	= species quantity
$()_e$	= edge of boundary layer
$()_d$	= dimensional quantity
$\bar{()}$	= mean value
$()'$	= disturbance value
$()_{el}$	= electronic value
$()_v$	= vibrational-electronic value
$()_{tr}$	= translational-rotational value
(N)PSE	= (Nonlinear) Parabolized Stability Equations
LST	= Linear (or Local) Stability Theory
CP, TP	= calorically, thermally perfect gas
CTE	= chemical and thermal equilibrium
CNE	= chemical nonequilibrium with thermal equilibrium
TNE	= Thermochemical Nonequilibrium

II. Introduction

HYPersonic boundary layer transition is critically important to hypersonic vehicle design due to its influence on heat transfer rates. Prediction of heat transfer informs the design of the Thermal Protection System (TPS), which is a significant portion of the mass of reentry vehicles, planetary probes, and Martian entry vehicles. Reducing this mass has benefits in terms of decreased fuel requirements and increased payload; however, due to the high risk and uncertainty, the TPS or heat shield is often designed conservatively assuming fully turbulent flow. Laminar flow results in reduced heat flux, and so more accurate and reliable prediction of transition should result in more efficient vehicle design. Limited previous research exists examining the problem of transition prediction for Martian atmospheric entry, with literature available on transition on the Mars Science Laboratory (MSL). Although transition was demonstrated in wind-tunnel tests [? ?], flight data [?], and numerical studies [? ?], uncertainty in the transition location was held to be high enough that the TPS should be designed for fully turbulent flow, and therefore, greater mass than would have been required for a partially-laminar TPS design.

Although Mach number and Reynolds number, based on momentum thickness, are commonly used for developing correlations to predict transition points, and have been used in previous studies for Martian entry applications, these correlations require a significant amount of data in order to be developed, and there is a large degree of uncertainty in applying such a correlation to situations outside of the specific wind tunnel or geometry used to gather the data. By contrast, the Linear Stability Theory (LST), sometimes also referred to as Local Stability Theory, linear Parabolized Stability Equations (PSE), and Nonlinear PSE (NPSE) methods provide a physics-based analysis of the boundary layer stability. These e^N methods are semiempirical due to requiring knowledge of the critical N-Factor for transition onset, and in the case of NPSE the initial disturbance amplitude is required. Saric et al. [?] reviewed the instability mechanisms that lead to laminar-turbulent transition, which can be categorized as streamwise (Mack first and second

modes), crossflow, centrifugal (Görtler), and attachment-line.

Predicting the exact point of transition is a difficult task that requires not only detailed analysis of boundary layer stability, but also detailed knowledge of the disturbances that will be encountered. Under most situations, the exact point of transition cannot be predicted due to a lack of knowledge about the freestream disturbances. The accepted practice is to reduce the N-Factor of a vehicle design in order to delay transition and improve the performance through a reduction of the percentage of the surface impacted by turbulent flow, despite not knowing the exact point of transition.

Chemical and thermal nonequilibrium are relevant to reentry applications because under hypersonic conditions the temperature within the boundary layer and behind strong shocks can rise above the point where molecular dissociation and chemical reactions will occur. At high enough temperatures, ionization reactions are possible, and in the case of ablative Thermal Protection Systems (TPS), the ablating material may react with the surrounding atmosphere, with the reaction mechanism depending on the chemical composition of the material. In order to accurately model the aerodynamics and boundary layer stability of this system, the chemistry effects must be taken into account. The presence of transitional flow, and the difficulty of accurately predicting the point of transition, is a major source of uncertainty, particularly for predicting heating [?] for hypersonic vehicles. Some of the options for modeling chemical and/or nonequilibrium effects include assuming a calorically or thermally perfect gas (CP or TP), incorporating the effects of chemical composition but assuming both chemical and thermal equilibrium (CTE), assuming thermal equilibrium but including chemical nonequilibrium (CNE), or thermochemical nonequilibrium (TNE).

A number of analytical studies focusing on hypersonic boundary layer transition neglecting chemistry effects are available in the literature [? ? ? ? ?], as well as experimental studies that use sufficiently low temperatures to avoid significant chemical reactions [?]. Relatively fewer studies that include chemistry effects are available [? ? ? ? ?]. Chemical equilibrium, chemical nonequilibrium or finite-rate chemistry, and thermochemical nonequilibrium have been compared in the past [? ? ? ? ?]. There are a number of recently-developed options for more advanced chemical models than will be addressed here, for example Jaffe et al. [?], Armenise et al. [?], Singh et al. [?] and Chaudhry et al. [?]. The code used in this work has been developed with the intention of being compatible with any user-provided chemical model, and while further investigation on the effects of the chemical model are outside the scope of this work, it has been shown that nonequilibrium chemistry is sensitive to the models used, and that boundary layer stability specifically is sensitive to vibrational energy relaxation as shown by Bertolotti [?] and touched on briefly in Figure 5 of Kline et al. [?].

Schneider [?] reviewed the available literature on laminar-turbulent transition for blunt body and capsule geometries, including Martian probe atmospheric entry, and MSL. In Ref. [?], Schneider discusses how transition over reentry shields is critical both for increasing the available payload through decreasing TPS thickness and for predicting and avoiding high, localized heating from aft-body boundary layer reattachment. Kimmel [?] provides a thorough review of hypersonic transition control techniques, and states that one of the difficulties of hypersonic transition control is that the techniques applied at lower speeds cannot be extrapolated to the high heating environment and the physical phenomena occurring within these boundary layers. At the same time, the potential benefits of a greater understanding of hypersonic boundary layer transition are significant. Analysis of the National AeroSpace Plane (NASP) aerodynamics [?] estimated that the possible payload of an air-breathing single-stage-to-orbit vehicle would double if it was fully laminar as compared to fully turbulent. Techniques to control transition include wall cooling, which is effective in stabilizing the first Mack mode but destabilizing to the second mode [? ?].

A number of studies have been conducted concerning the Mars Science Laboratory (MSL) entry vehicle aerothermodynamics. Edquist et al. [?] conducted detailed computational studies of the MSL, focusing on thermal and chemical nonequilibrium with an eight-species gas mixture, using Park [?] reaction rates and using a critical value of momentum-thickness Reynolds number. The peak turbulent heating rate was predicted to be 70% higher than the heating rate for laminar flow, with a fully turbulent shield experiencing 38% higher integrated heat load as compared to the fully laminar case. Hollis et al. [? ?] compared laminar, transitional, and turbulent heating data on the MSL entry vehicle in an air wind tunnel and a high-enthalpy shock tunnel with CO_2 gas, and compared results to Navier-Stokes solutions. Using laminar CFD solutions, they produced transition location correlations based on boundary layer momentum thickness, edge Mach number, and Reynolds number based on momentum thickness. Selected cases from these wind tunnel tests have been analyzed with the Langley Stability and Transition Analysis Code (LASTRAC) [?] by Chang et al. [?] with air. Johnson et al. [?] conducted similar analyses using PSE analysis for nonequilibrium air, and initial analysis for nonequilibrium CO_2 . Although not applied to Martian entry applications, experimental and computational work has been done investigating a stabilizing effect of CO_2 injection into high enthalpy boundary layers for delay of transition [? ? ?], due to the characteristic of CO_2 to absorb energy at frequencies close to the second Mack mode.

In this work, we analyze the boundary layer stability of a reentry vehicle at an angle of attack, with freestream

conditions drawn from circumstances in literature where transition was suspected either in wind tunnel experiments or in flight. This work builds on previous works by Kline et al. [?] in which the authors developed the thermochemical nonequilibrium capabilities for LASTRAC [?] and applied them to various conditions including a $CO_2 - N_2$ mixture approximating the Martian atmosphere. LASTRAC [?] is a boundary layer stability analysis code that provides PSE as well as LST to predict the stability of a boundary layer and transition with semiempirical e^N methods. The thermochemical capabilities have since been extended to three-dimensional geometries in previous work [?]. This previous work analyzed the same geometry using LST at a single flow condition, which we now analyze at multiple flow conditions using PSE in order to observe whether the trends in N-factor are consistent with the experimental results.

III. Methodology

The LASTRAC solver has recently been modified to allow chemical nonequilibrium in thermal equilibrium (CNE), chemical and thermal equilibrium (CTE), and thermochemical nonequilibrium (TNE) air gas chemistry. These capabilities are required for hypersonic boundary layer transition prediction since at the high temperatures experienced by hypersonic vehicles air can no longer be assumed a perfect gas, and the chemical and thermochemical nonequilibrium effects should be taken into account. In this work, we further extend this capability to Martian atmosphere gas chemistry. Section A will describe the PSE method, followed by a description of the chemical model in Section B. In this work, a 5-species mixture of CO_2 , O_2 , O , C , and CO , is used in order to model a flow with a freestream mass fraction of 100% CO_2 which may dissociate due to high temperatures.

A. Boundary Layer Stability Analysis

LASTRAC includes capabilities to analyze boundary layer stability with LST and PSE. These methods assume a disturbance vector solution that is a discrete sum of a Fourier series. The LST method assumes that the boundary layer is nearly parallel, with negligible growth of the thickness of the boundary layer, and uses a mode shape, or perturbation form, for the Fourier series that has a shape function and wave number that are locally constant in the streamwise direction. For the PSE, the assumed mode shape uses a shape function and wave number that vary slowly in the streamwise direction. While an eigenvalue problem is formed in the LST approach, the PSE method numerically solves an approximate form of the governing partial differential equations for the slow-varying shape function with an actively updated wave number along the streamwise direction. The nonlinear PSE uses a mode shape similar to the PSE, but retains nonlinear terms from the Navier-Stokes equations, and requires a known finite disturbance while both LST and linear PSE are independent of the input disturbance amplitude but only valid for sufficiently small disturbances. LASTRAC was modified to include further capabilities for high-enthalpy hypersonic applications by Kline et al. [?]. Further details on the capabilities previously available in LASTRAC are available in the LASTRAC manual [?]. Previous work [?] includes more complete details of the modifications required to accommodate gas chemistry effects.

Stability equations are derived starting from the nondimensionalized Navier-Stokes equations. A body-fitted coordinate system is used where x , y , and z are defined as streamwise, wall-normal, and spanwise, respectively. Perturbations to the mean flow quantities are expressed in terms of the disturbance vector $\phi = \{p', u', v', w', T'\}^T$. The disturbance field ϕ is assumed to be periodic in space and time, and so the disturbance vector can be expressed as a Fourier series,

$$\phi(x, y, z, t) = \sum_{m=-M}^M \sum_{n=-N}^N \chi_{mn}(x, y) e^{i(n\beta z - m\omega t)}, \quad (1)$$

where M and N represent the numerical resolution in time and space, respectively. The fundamental temporal wave number is a nondimensionalized form of the physical frequency f , $\omega = \frac{2\pi \ell}{u_e} f$. Substituting a single disturbance mode defined by the wave number ω and spanwise wave number $\beta = \frac{2\pi}{\lambda_z}$ in Equation 1 results in the Linearized Navier-Stokes (LNS) equation.

This equation can be solved numerically, and simplifications lead to approximate solutions that are obtained at a lower computational cost for engineering applications. One such simplification is the quasiparallel assumption that neglects the velocity normal to the wall and all mean flow variation in the x direction. The linear PSE decomposes the mode shape into two parts: a complex wave number α that varies only in x and a shape function that varies in x and y ,

$$\chi = \hat{\chi}(x, y) e^{i \int_{x_0}^x \alpha(\xi) d\xi}, \quad (2)$$

where ξ is the variable of integration. The linear PSE neglects the products of disturbances, or 2^{nd} - and higher-order perturbations. Another possible simplification is the quasiparallel assumption that neglects velocity normal to the wall

and all mean flow variation in the x direction, where χ is a function of y only, leading to the LST solutions. This process is repeated separately for the CP, CTE, CNE, and TNE models.

The methods described above to solve for ϕ produce results presented in terms of a nondimensional frequency F , the complex part of the wavenumber α_i , and the N-Factor based on disturbance kinetic energy,

$$\begin{aligned} F &= \frac{2\pi\nu_e}{u_e^2} f \\ \alpha_i &= \Im(\alpha(x)) \\ E &= \int_0^{y_e} \rho(|u'|^2 + |v'|^2 + |w'|^2) dy \\ \sigma(x) &= -\alpha_i(x) + \frac{1}{2E} \frac{dE}{dx} \\ N(x) &= \int_{x_0}^x \sigma(\xi) d\xi = \log\left(\frac{A}{A_0}\right). \end{aligned} \quad (3)$$

The N-Factor, N , refers to the logarithm of the amplitude change of a disturbance with initial amplitude, A_0 , calculated using the integrated growth rate, σ , based on disturbance kinetic energy, E , which is evaluated to the edge of the boundary layer, y_e . The integral defining N is evaluated with the neutral point where the imaginary growth rate first becomes positive as the lower bound. The critical N-Factor (N_{crit}) is the value of the N-Factor where transition would be expected to occur based on experimental correlations. When α_i is negative the associated eigenmode is unstable.

For CNE or TNE models, additional equations are necessary to calculate the species mass fractions and their disturbances. The continuity and momentum equations remain unchanged, using mixture values for ρ , p , and μ . Equations governing species production and destruction are added, and the energy equation must be updated to include energy changes from the chemical reactions. These equations can be found in works by MacCormack and Candler [?], Chang et al. [?] and Anderson [?]. Mixture terms are required as functions of the species properties,

$$\begin{aligned} C_p &= \sum_{s=1}^{N_s} C_s C_{p,s} \\ \rho &= \sum_{s=1}^{N_s} \rho_s = \frac{p}{R_u \sum \frac{C_s}{M_s} T} \\ C_s &= \rho_s / \rho, \quad \sum C_s = 1 \\ \dot{\omega}_{s,d} &= M_s \sum_{r=1}^{N_r} (\beta_{s,r} - \alpha_{s,r}) (R_{f,r} - R_{b,r}) \\ \dot{\omega}_s &= \dot{\omega}_{s,d} \frac{\ell}{\rho_e u_e}, \end{aligned} \quad (4)$$

where M_s is the species molar mass, R_u the universal gas constant, ρ_s is the species density, N_s is the number of species in the gas mixture, $\dot{\omega}_s$ represents the nondimensionalized species production rate due to chemical reactions, D_s is the diffusivity of species s with respect to the gas mixture normalized by the value at the boundary layer edge D_e , and h_s is the enthalpy per unit mass of species s nondimensionalized by edge temperature and heat capacity. The terms $\beta_{s,r}$ and $\alpha_{s,r}$ are the stoichiometric coefficients for the N_r reactions being considered, and $R_{f,r}$ and $R_{b,r}$ are the associated reaction rates. The disturbance vector now includes species mass fractions, $C_s = \bar{C}_s + C'_s$.

In the previous equations, thermal equilibrium was assumed. This means that the vibrational, electron, translational, and rotational energies had equilibrated and a single temperature is sufficient. *In other words, we assume that the relaxation time between these energy modes is sufficiently shorter than the time scale of the flow phenomena. This is not necessarily true for hypersonic problems.* For thermal nonequilibrium, multiple temperatures are required. In this work, we will use a two-temperature model for TNE, where the vibrational-electronic energies are associated with $T_V = T_{vib} = T_{el}$, where T_e refers to the electron translational-rotational temperature. The translational-rotational energy for all other species is associated with $T = T_{trans} = T_{rot}$. As compared to thermal equilibrium with CNE, an additional equation and variable are added to the system, with the associated disturbance T'_V . In addition, the chemistry model will take into account different rate controlling temperatures based on T and T_V depending on what type of reaction is occurring.

The total energy equation is updated,

$$\begin{aligned} \rho C_p \left[\frac{\partial T}{\partial t} + (\vec{V} \cdot \nabla) T \right] + \rho C_{p,v} \left[\frac{\partial T_V}{\partial t} + (\vec{V} \cdot \nabla) T_V \right] = \frac{1}{RePr} \nabla \cdot (k \nabla T + k_v \nabla T_V) + Ec \left(\frac{\partial p}{\partial t} + (\vec{V} \cdot \nabla) p \right) \\ + Ec \frac{\Phi}{Re} + \frac{Le}{RePr} \sum_{s=1}^{N_s} \left(\nabla(h_s) \cdot (\rho D_s \nabla C_s) \right) + \sum_{s=1}^{N_s} h_s \dot{\omega}_s, \end{aligned} \quad (5)$$

and a vibrational-electronic energy equation is added:

$$\begin{aligned} \rho C_{p,v} \left[\frac{\partial T_V}{\partial t} + (\vec{V} \cdot \nabla) T_V \right] = \frac{1}{RePr} \nabla \cdot (k_v \nabla T_V) + Ec \left(\frac{\partial p_{el}}{\partial t} + (\vec{V} \cdot \nabla) p_{el} \right) \\ + \frac{Le}{RePr} \sum_{s=1}^{N_s} \left(\nabla(h_{v,s}) \cdot (\rho D_s \nabla C_s) \right) \\ + \sum_{s=mol} \rho_s \frac{(e_{v,s}^* - e_{v,s})}{< \tau_s >} + 2\rho_{el} \frac{3}{2} \bar{R}(T - T_V) \sum_{s=1}^{N_s-1} \frac{\nu_{es}}{M_s} - \sum_{s=ions} \dot{n}_{e,s} \hat{I}_s + \sum_{s=1}^{N_s} \dot{\omega}_s \hat{D}_s, \end{aligned} \quad (6)$$

where the T_V is normalized by the boundary layer edge value of the translational temperature T_e , $C_{p,v}$ is the constant pressure specific heat for electron-vibrational energy modes and $\int_0^{T_V} C_{p,v} dT = e_v$, the combined electron and vibrational energy. $C_{p,v}$ is normalized by the edge specific heat $C_{p,e}$, and the remaining terms are similarly nondimensionalized. The vibrational thermal conductivity k_v , vibrational-translational relaxation time $< \tau_s >$, species vibrational enthalpy $h_{v,s}$, vibrational energy per unit mass of diatomic molecules $\hat{D}_s$ have been added, and are provided by the chemistry model. In this work, electron and ion species are not included, and so ionization and electron related terms such as the electron pressure p_{el} , collision frequency between electrons and neutral particles ν_{es} , rate of ion production $\dot{n}_{e,s}$ and ionization energy $\hat{I}_s$ will not be needed.

B. Chemical Rates and Thermodynamic Properties

A number of the quantities needed for boundary layer stability are dependent on the gas composition, including species production rates $\dot{\omega}_s$, transport properties viscosity and thermal conductivity, and thermodynamic quantities of specific heats and enthalpy. The equations implemented in LSTRAC to accommodate these models have been described previously [?]. This section will summarize which models were selected and address the relaxation time model.

The chemistry model used in this work is similar to that developed by Thompson et al. [?] for the calculation of thermodynamic and transport properties, with modifications to the curve fits used and additional data introduced to accommodate Martian atmospheric composition. The chemistry model used in this work uses the Chemical Equilibrium with Applications (CEA) format for thermodynamic curve fit coefficients, with the equations for specific heat, enthalpy, and entropy for each species from McBride et al. [?]. The constants for this curve fit are available from Ref. [?].

In addition to the thermodynamic quantities, transport quantities of viscosity, thermal conductivity, and diffusion coefficients are required. These quantities are calculated as functions of collision integrals between all pairs of chemical species included in the model. The collision integrals or collision cross-sections $\pi \tilde{\Omega}_{i,j}^{(l,s)}$ for momentum transfer are defined as integrated functions of the differential cross section for the pair of species, the relative velocity and reduced velocities of the colliding particles, and the scattering angle. This equation can be found in Yos [?], and rather than evaluate the detailed expression for the collision cross-section at each temperature, curve fits based on cross-section values evaluated at a range of temperatures are used commonly in literature [? ?]. A curve fit for air is available from Gupta et al. [?].

Coefficients for curve fits for a CO_2 -based mixture were calculated using tabulated values from Wright et al. [?], using minimization of the mean square difference with the tabulated values. According to collision integral data tabulated by Wright [?], the uncertainty in the values of the collision integrals ranges anywhere from $\pm 5\%$ to $\pm 50\%$, and so although a curve fit can match the data closely, it should not be expected to be any more accurate than the data used.

The modified Arrhenius equations are used to calculate reaction rates used to produce the species production rate $\dot{\omega}$, with the rate-controlling temperature T_c determined by the type of reaction. $T_c = \sqrt{TT_V}$ as used by Park [? ?] for dissociation reactions and $T_c = T$ for heavy molecule collision reactions. In this work, the coefficients for the modified

Arrhenius equations are drawn from Park [?]. Noncatalytic boundary conditions are used at the surface in both mean flow and disturbance equations. Although ionization and radiation effects are expected to be significant for reentry applications, these effects are neglected in the current work due to the increased complexity and computational cost. These effects may be included in the future. Effects of ablation and chemical reactions with ablation products are also neglected. Ionization, ablation, and three-temperature models are outside the scope of this work, where the next reasonable step to increase complexity and accuracy would be the addition of ionization effects.

The vibrational-translational energy relaxation time for diatomic molecules is found using the Millikan-White correlation [?] and a collision cross-section correction by Park [?]:

$$\begin{aligned} \langle \tau_s \rangle &= \tau_s^{MW} + \begin{cases} \tau_s^P & T > 8000 \text{ K} \\ 0 & T < 8000 \text{ K} \end{cases} \\ \tau_s^{MW} &= \frac{1}{p_{atm}} \frac{\sum_{i=1, \neq e^-}^{N_s} n_i e^{A_s (T^{1/3} - 0.015 \mu_{si}^{1/4}) - 18.42}}{\sum_{i=1, \neq e^-}^{N_s} n_i} \\ \tau_s^P &= (\sigma_s \bar{c}_s n_s)^{-1} \\ \bar{c}_s &= \sqrt{(8k_B T / \pi (M_s / Av))}, \end{aligned} \quad (7)$$

where τ_s^{MW} is the Millikan and White [?] semiempirical correlation, and τ_s^P is the Park [?] correction, using $\sigma_s = 10^{-16} \text{ cm}^2$ as used by Gnoffo [?], Av is Avogadro's number such that M_s / Av is the mass per particle of species s in kg , and $n_s = C_s / M_s$ is the number density per species. Unlike [?], we use τ_s directly rather than an averaged term. For TNE flow, the state equation should also be updated in the presence of electrons:

$$p = \sum_{s=1, s \neq e^-}^{N_s} \left(\rho_s \frac{R_u}{M_s} T \right) + \rho_{el} \frac{R_u}{M_{el}} T_V, \quad (8)$$

where in this work electron species are not included, and this reduces to the previously-used state equation. The final term of Equation 6 represents the production of vibrational energy due to the creation and destruction of diatomic molecules with the vibrational energy per unit mass of the molecules represented by $\hat{D}_s$. The approximation suggested by Park [?], $\hat{D}_s = \bar{D}_s - k_B T$, is used with the dissociation energy $\bar{D}_s$ taken from tabulated values. This makes the assumptions that there is preferential dissociation and recombination of the molecules in the higher vibrational states, and that the vibrational energy removed by dissociation differs by the average translational energy.

For molecules with multiple vibrational modes, specifically CO_2 , we should instead use a form of the Landau-Teller equation based on the number of vibrational modes and the characteristic vibrational temperatures. The relaxation time for a species s given vibrational mode j with characteristic temperature θ_j and reduced mass $\mu_{s,k}$ of the species and the colliding molecule k from Millikan and White [?] using Landau Teller theory is,

$$\ln(p\tau_{s,j,k}) = (1.16 \times 10^{-3}) \mu_{s,k}^{\frac{1}{2}} \theta_j^{\frac{4}{3}} \left(T^{\frac{-1}{3}} - 0.015 \mu_{s,k}^{\frac{1}{4}} \right) - 18.42, \quad (9)$$

where we take the averaged relaxation time for vibrational mode j of species s in a mixture of N_s species as:

$$\tau_{s,j} = \sum_{k=1}^{N_s} (\tau_{s,j,k} \rho_k) / \sum_{N=1}^{n_s} \rho_k. \quad (10)$$

The vibrational-translational relaxation term from Equation 6 requires the vibrational energy term $e_{v,s} = \int_0^{T_V} C_{v,v}^s dT$ and this same term taken if the vibrational-electronic temperature was set equal to the translational-rotational temperature, $e_{v,s}^*$.

The vibrational specific heat can be expressed in terms of the energy mode characteristic temperatures as:

$$C_{v,v}^s = \frac{R_u}{M_s} \left(\frac{\theta_j}{T} \right)^2 \frac{e^{(-\theta_j/T)}}{(1 - e^{(-\theta_j/T)})^2}. \quad (11)$$

Taking the integral to find the internal energy, for N_v vibrational modes with degeneracy g_j ,

$$\frac{e_{v,s}^* - e_{v,s}}{\langle \tau_s \rangle} = \sum_{j=1}^{N_v} \frac{g_j \theta_j}{\tau_{s,j}} \frac{R_u}{M_s} \left(\left(e^{\left(\frac{\theta_j}{T} \right)} - 1 \right)^{-1} - \left(e^{\left(\frac{\theta_j}{T_V} \right)} - 1 \right)^{-1} \right). \quad (12)$$

Table 1 Flow conditions from Ref. [?] for three transitional wind tunnel cases.

Case	U_∞ [m/s]	T_∞ [K]	P_∞ [Pa]	ρ_∞ [kg/m ³]	$Re_{D,\infty}$	M_∞
LENS-XX Shot 18	2021	140	614	0.0232	1.38E+06	10.7
LENS-XX Shot 19	3080	290	440	0.00801	3.40E+05	11.6
LENS-XX Shot 08	3834	435	628	0.00765	2.87E+05	12

IV. Results

Section A describes the flow conditions and the mean flow solution results. Section B describes LST results at a fixed location used to determine appropriate ranges of instabilities to investigate with PSE in Section C.

A. Mean Flow Solutions

Table 1 summarizes the free stream flow conditions used in this work. All cases use a pure CO₂ freestream gas, are at an angle of attack of 16°, and a wall temperature of 300 K with noncatalytic and isothermal boundary conditions. The model used in wind-tunnel tests was an 8-in. diameter 70 degree sphere-cone model similar to the Mars Science Laboratory (MSL) entry vehicle and described more fully in Hollis et al. [? ?].

LAURA version 5.5-65135 [?] was used to produce the three-dimensional mean flow solutions, using a multiblock structured mesh. To produce mean flow solutions appropriate for boundary layer stability analysis, mesh dimensions with 257 points normal to the surface were used, based on the mesh convergence shown in Chang et al. [?]. The mesh adaptation to capture the shock and initial adaptation to the boundary layer thickness uses LAURA built-in adaptation utilities, and a further custom mesh adaptation was then applied to achieve a boundary layer mesh distribution appropriate to boundary layer stability calculations. This adaptation incorporated 150 points within the boundary layer, with a grid distribution that uses 30 points with constant spacing in the first 10% of the boundary layer adjacent to the wall, smoothly transitioned to a second region of constant spacing through the remainder of the boundary layer. For stability calculations, the flow solution is interpolated to boundary layer profiles normal to the surface at points defined on a one-block, 401x201 surface mesh. This analysis proceeds similarly to that of by Chang et al. [?]. The gas chemistry model described in the previous section applies to the stability analysis, which differs somewhat from the models used in LAURA 5. The effect of these differences is neglected in this work.

Figure 1 illustrates the temperature contours at Shot 08 conditions. This figure also identifies point A, which is used for local stability solutions in later sections. Although the three-dimensional flow, using one-half the geometry split along the symmetry plane, is evaluated in this work, due to low crossflow Reynolds numbers, which are less than 50 across the entire surface, no crossflow instabilities are expected and so we analyze only the symmetry plane.

B. Local Stability Analysis with Optimized Spanwise Wave Angle

This section compares the LST results at point A illustrated in Figure 1. These results use the optimized wave angle capabilities of LASTRAC to find the spanwise wave length producing the maximum growth rate for a given instability wave frequency. The results for Shot 18 and Shot 19 are illustrated in Figures 2 and 3. Figure 2 compares the optimized growth rates and streamwise wave numbers at point A. These results are used to provide the range of frequency and spanwise wave lengths used to execute the PSE analysis. Figure 3 compares the spanwise wave angle and phase speeds. For both plots, the color is used to indicate the variable being plotted, while the line style is used to indicate the flow condition. From these plots, it appears that the same instability mechanism is at play in each case. We can see that at this location, while there is a slight oblique angle at low frequencies, a nearly two-dimensional mode is more dominant. The boundary layer edge Mach numbers at this location are 1.46 for shot 08, 1.31 for shot 18, and 1.67 for shot 19. Figure 4 illustrates the eigenfunction profiles at point A for shot 19, at frequencies chosen to illustrate how the mode shape is changing across the frequency range.

C. PSE Analysis

This section compares PSE results for the three flow conditions described in Section A. Based on the LST results of Section B, a range of frequencies and spanwise wave lengths were used with the linear PSE analysis with a TNE model in LASTRAC. The resulting N-Factor envelopes are overlaid in Figure 5b. Figure 5 compares experimental results from Hollis et al. [?] to the N-Factor envelopes resulting from the PSE analysis conducted on the three wind tunnel

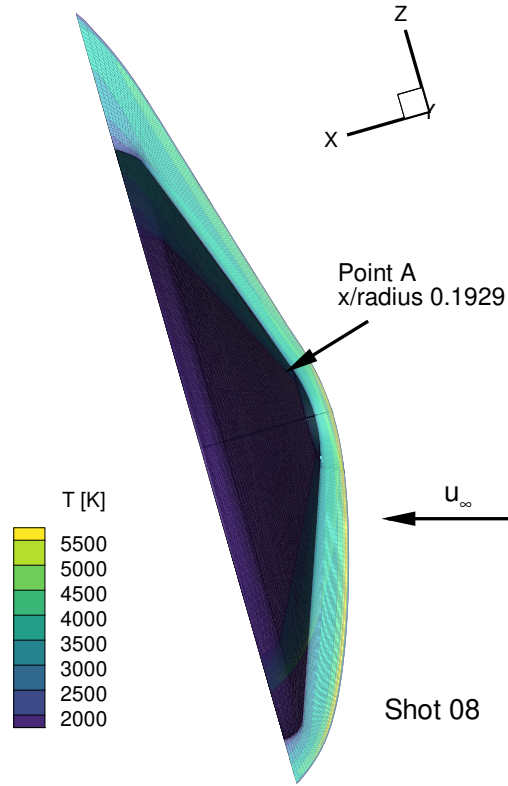


Fig. 1 Contours of translational temperature for the highest-enthalpy case (shot 08), illustrating the symmetry plane at a 16° angle of attack. Point A is included for reference in later plots.

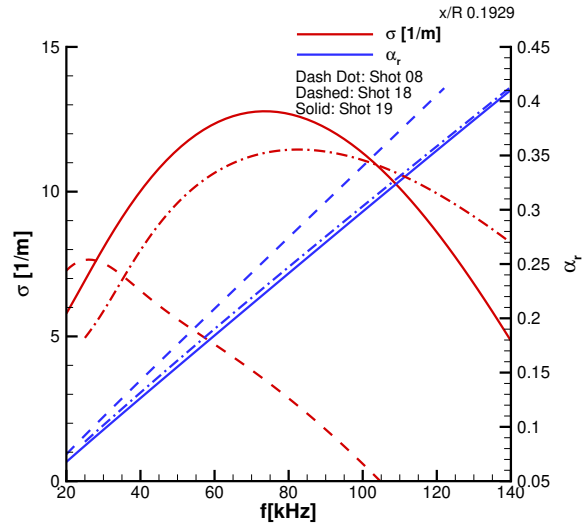


Fig. 2 Local growth rate and nondimensional streamwise wave number for shots 08 (dash-dot), 18 (dashed) and 19 (solid) at point A shown in Figure 1.

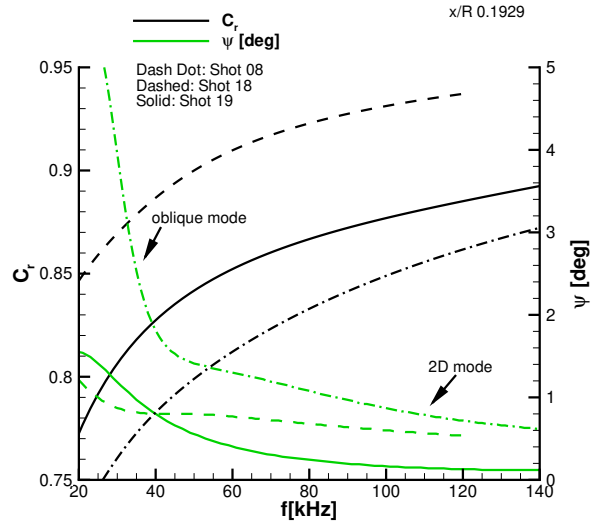


Fig. 3 Phase speed and spanwise wave angle for shots 08 (dash-dot), 18 (dashed) and 19 (solid) at point A shown in Figure 1.

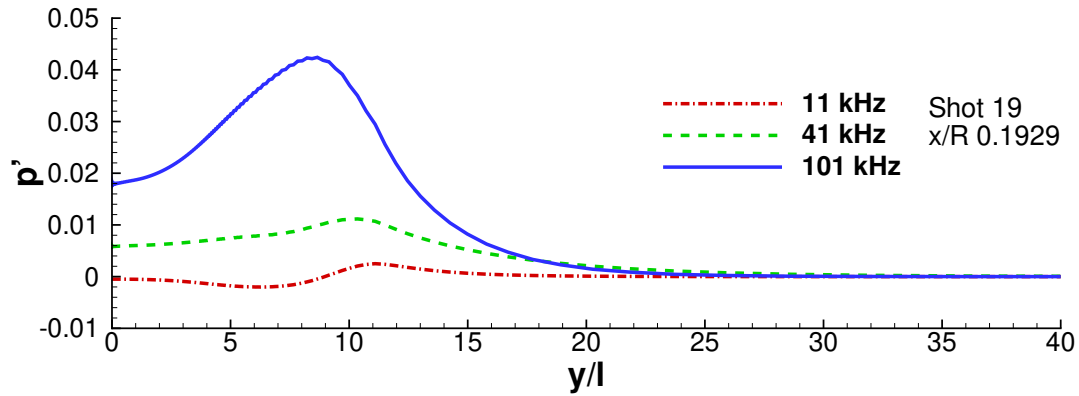


Fig. 4 Pressure perturbation mode shapes at $x/R = 0.1929$, for shot 19.

conditions. In Figure 5a, the thermocouple and thin film data from these three cases are overlaid with dashed lines indicating possible points of transition. Determining a precise transition location from the experimental data is difficult due to relatively large error bars, and only some cases match well with the laminar solution on the windward side from the CFD prediction included in Ref. [?]. We choose the first point where there is a sharp rise in the surface heating, indicated by dashed lines in Figure 5a.

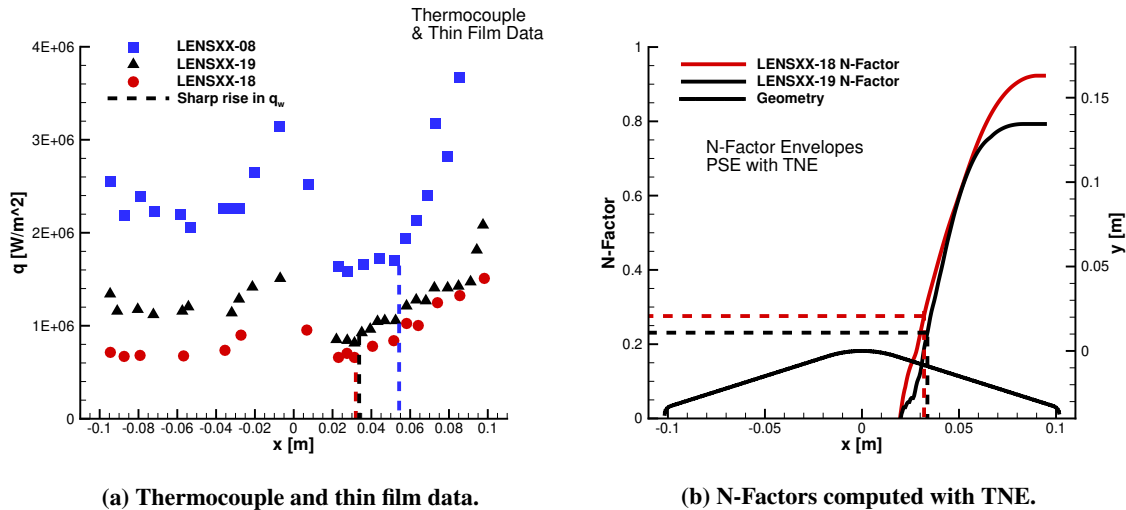


Fig. 5 Experimental results from Hollis et al. [?] compared against current work, cases LENSXX shot 18 and shot 19.

Comparing these transition points against the N-Factor envelopes in Figure 5b, we can see that there is a critical N-Factor of under 0.3. This critical N-Factor is significantly lower than the critical N-Factor of 4 normally associated with wind-tunnel experiments. PSE analysis of shot 08 did not find any instability waves along the symmetry plane, although LST analysis indicates that there was a weak instability. The wave angles of the individual PSE solutions producing the maximum N-Factor at and further downstream of the transition point are around 60° for shot 18 and around 85° for shot 19, indicating an oblique first-mode instability. The extremely low N Factors at experimentally measured transition locations indicate that the mean flows computed for all three cases are very stable to small perturbations. The discrepancy with experiments could be due to inaccuracies and assumptions in thermochemistry models, or due to a mismatch between the boundary conditions of noncatalytic isothermal walls and 100% CO_2 and what actually occurred under experimental conditions. These sources of uncertainty may be addressed through either repeating the analysis with improved and more refined mean flow solutions, through evaluating sensitivity to chemical models, or through using methods that address finite disturbances such as NPSE or DNS. However, it is arguably more likely that transition was caused by a different instability mechanism such as nonmodal growth [? ?] or roughness-induced transition [?]. Whether transition is in fact caused by a different instability mechanism, or an explanation for why such a low N-Factor would cause transition, is left for future work.

V. Conclusions

This work investigated the boundary layer stability of a Mars atmosphere entry vehicle at angle of attack, at freestream conditions drawn from literature. A small number of cases in literature indicate transitional flow for CO_2 -gas mixtures under high-enthalpy conditions. With LASTRAC 3.1, we are now able to evaluate the boundary layer stability under these conditions including thermochemical nonequilibrium. The mean flow solutions used in this work may have been insufficiently resolved. This is just one of several sources of uncertainty for the instability results presented in this work, including uncertainties in matching experimental conditions, and modeling approximations for terms such as the vibrational-translational relaxation time and reaction rates. Given higher fidelity flow solutions, or experimental measurements allowing more certainty in the freestream conditions, we would expect the frequencies and growth rates of the instabilities to shift, however, the overall character of the instabilities would be expected to remain, in the absence of large roughness or freestream disturbances.

The tools implemented in previous work allow analysis of the boundary layer stability in a Martian atmosphere [? ?]. In this work, these tools were applied to MSL wind tunnel cases where transition was observed or suspected under experimental conditions in an attempt to explain the transitional behavior. This required the three-dimensional and thermochemical nonequilibrium capabilities of LSTRAC. Three-dimensional boundary layer stability analysis was available in a previous version of LSTRAC for calorically or thermally perfect gases only. The pure- CO_2 wind tunnel conditions were modeled as a 5-species mixture of CO_2 , O_2 , O , C , and CO . Transport properties in the reacting mixture of thermally perfect gases were modeled using collision integral curve fits from literature. Ablation, radiation, and ionization, although relevant to Martian atmospheric entry, will be neglected in this work as they are not yet incorporated in LSTRAC.

Instabilities were found along the symmetry plane of this geometry, with a nearly two-dimensional mode being dominant from LST analysis at a point upstream of transition, while from PSE analysis an oblique mode produced first mode instabilities that resulted in the maximum N-Factor further downstream at the transition location. Comparing PSE results against experimental results indicated transition occurring at very low N-Factor values, on the order of 0.3. This indicates that further study is needed, either through continuing this analysis with consideration of the potential uncertainties mentioned above, or through examining nonmodal instabilities, which may occur on blunt geometries as investigated by Paredes et al.[? ?]. Despite not explaining transition on the MSL geometry in this work, we are able to show a capability to evaluate thermochemical nonequilibrium boundary layer stability with nonparallel and three-dimensional effects in CO_2 ; this capability may now be applied to other circumstances, potentially including the flight conditions for MSL atmospheric entry.

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