Numerical Simulation of Hypersonic Boundary-Layer Instability in a Real Gas with Two-Dimensional Surface Roughness

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Experimental and numerical results have shown that two-dimensional surface roughness can stabilize a hypersonic boundary layer dominated by second-mode instability. It is sought to understand how this physical phenomenon extends from an airflow under a perfect gas assumption to that of a real gas. To these ends, a new high-order shock-fitting method that includes thermochemical nonequilibrium and a cut-cell method to handle complex geometries unsuitable for structured body-fitted grids is presented. The new method is designed specifically for direct numerical simulation of hypersonic boundary-layer transition in a hypersonic real-gas flow with arbitrary shaped surface roughness. The new method is validated and shown to perform comparably to a high-order method with a body-fitted grid. For a Mach 10 flow over a flat plate with a real-gas model, a two-dimensional roughness element was found to stabilize the second mode when placed downstream of the synchronization location which is consistent with previous research for perfect-gas flows. For a Mach 15 flow over a flat plate, a two-dimensional surface roughness element stabilizes the second-mode instability more effectively in a real gas than in a perfect gas.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>−αi</td>
<td>Growth rate</td>
</tr>
<tr>
<td>c_r</td>
<td>Phase velocity</td>
</tr>
<tr>
<td>c_s</td>
<td>Mass fraction of species s</td>
</tr>
<tr>
<td>e_v,s</td>
<td>Species specific vibration energy, J/kg</td>
</tr>
<tr>
<td>h</td>
<td>Roughness height, m</td>
</tr>
<tr>
<td>h_o,s</td>
<td>Species heat of formation, J/kg</td>
</tr>
<tr>
<td>M_s</td>
<td>Species molecular weight, kg/mol</td>
</tr>
<tr>
<td>p</td>
<td>Pressure, N/m²</td>
</tr>
<tr>
<td>Q_{T-V,s}</td>
<td>Species vibration energy transfer rate, J/m³·s</td>
</tr>
<tr>
<td>R</td>
<td>Universal gas constant, 8.3143 J/mol·K</td>
</tr>
<tr>
<td>T</td>
<td>Translation-rotation temperature, K</td>
</tr>
<tr>
<td>t</td>
<td>Time, s</td>
</tr>
<tr>
<td>T_V</td>
<td>Vibration temperature, K</td>
</tr>
<tr>
<td>u_j</td>
<td>Velocity in jth direction, m/s</td>
</tr>
</tbody>
</table>

nms Number of molecular species

ns Number of species

Subscripts

∞ Freestream

b Blowing/suction slot

s Species

w Wall

Symbols

δ Boundary layer thickness, m

δ_{ij} Kronecker delta

μ Viscosity, kg/m·s

ω_s Rate of species production, kg/m³·s

ρ Density, kg/m³

I. Introduction

Surface roughness has served primarily to promote early transition in a hypersonic flow when compared to a smooth surface, or, to not adversely affect transition significantly [1]. However, there has been some

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experimental evidence that surface roughness can delay the onset of transition in a hypersonic flow [2]. Also, recent direct numerical simulation results from [3, 4, 5, 6] have shown that judiciously placed two-dimensional roughness elements can actually stabilize a hypersonic boundary layer and delay transition onset. Following these findings, experiments were performed in [7] which showed that, indeed, similar to the direct numerical simulation results, two dimensional roughness elements can delay the onset of transition in a physical air flow. The fact that the numerical and experimental evidence is consistent brings the idea that perhaps a passive control strategy may be implemented in flight, using finite height roughness, to stabilize a hypersonic boundary layer.

It is commonly understood that the hypersonic transition process over flat plates and straight cones in a low disturbance environment follows certain paths. Initially, freestream disturbances are converted into boundary layer instabilities. In the absence of surface roughness, the amplification of linear wavelike disturbances, such as the second mode, leads to mode interactions and parametric instabilities. After which, there is a breakdown stage and finally turbulence. Eigenmode growth of linear wavelike disturbances is generally the slowest part of the transition process and the most unstable frequencies persist downstream. Common methods for modeling these linear wavelike disturbances are linear stability theory (LST), parabolized stability equations (PSE) and direct numerical simulation (DNS). These methods are designed to predict the growth or decay of wavelike disturbances based on a laminar meanflow profile. Much attention has been placed on studying the second mode as it has, in hypersonic laminar-turbulent transition, a strong impact on boundary layer transition. The second mode, for a fixed frequency, appears near the synchronization location of mode S and mode F. Mode S is named as it originates from the slow acoustic spectrum. Similarly, Mode F is named as it originates from the fast acoustic spectrum. As the phase velocities of these modes coincide, there is an energy exchange and the second mode appears from either mode S or mode F.

The potential delay of transition in a hypersonic boundary layer by two-dimensional roughness elements, as shown in [3, 4, 5, 6, 7], comes from the second mode being the most dominant instability mode. It was shown that a two-dimensional roughness element, that is less than the boundary-layer thickness, when placed after the synchronization point of mode S and mode F, can lead to a suppression, or stabilization, of the second mode. When the same roughness element is placed upstream of the synchronization point, the second mode is destabilized, i.e., the second-mode instability growth is higher. Therefore, the location of the roughness element is critical to achieving a delay in transition.

As the Mach number increases in a hypersonic flow, real gas effects become increasingly important. Higher energy modes, such as the vibrational energy of N$_2$ and O$_2$ in an air flow, can become excited and chemical reactions can occur in the flow due to high temperatures occurring downstream of the shock. These processes generally occur over a short time scale, which may be on the same order as the flow time scale, resulting in thermal and chemical nonequilibrium. These processes are not accounted for with an assumption of a perfect gas and can alter the instability of a hypersonic boundary layer. To capture these nonequilibrium processes, some sort of nonequilibrium model may be used. It was shown in [8], that real gas effects can significantly alter the instability characteristics of a hypersonic boundary layer and result in significantly different predictions in the location of transition onset depending on the gas model. The results of [3, 4, 5, 6] all used a perfect gas model to assess the effects of two-dimensional surface roughness on the second-mode instability in a hypersonic boundary layer. In this work, a thermochemical nonequilibrium model will be used study how a real gas is influenced by two-dimensional surface roughness.

The goals of this paper are 1) to validate a new high-order shock-fitting direct simulation method for hypersonic flows with thermochemical nonequilibrium and arbitrary surface roughness, and 2) to study, by DNS, the effects of two-dimensional roughness elements in a real-gas flow on hypersonic boundary-layer instability over a flat plate. A DNS study is required to capture the complex interplay of surface roughness and real-gas effects on boundary-layer instability. To simulate surface roughness, the cut-cell method developed in [9], will be implemented into an existing thermochemical nonequilibrium DNS code. The DNS code uses a five species gas model for air (N$_2$, O$_2$, NO, N, and O) to model chemical nonequilibrium and a two-temperature model to simulate thermal nonequilibrium. Two separate meanflow conditions at Mach 10 and Mach 15 are used to study the effects of surface roughness. Real-gas and perfect-gas flow simulations are performed for multiple roughness heights to find if the damping of the second mode by two-dimensional surface roughness follows the trends found in [3, 4, 5, 6] and how a real gas influences these trends.

The paper will start with an overview of the governing equations and the gas phase models followed by the numerical method for DNS using the cut-cell method. Next, the cut-cell method will be validated for a
geometry that can be simulated with either a body-fitted or a cut-cell grid. After the validation is performed, unsteady DNSs of a flat plate at Mach 10 and Mach 15 will be computed to assess how two-dimensional surface roughness elements affect second-mode instability when a real-gas model is used.

II. Governing Equations and Gas Phase Models

The governing equations for thermochemical nonequilibrium are formulated for a two-temperature model with the rotational energy mode assumed to be fully excited and five non-ionizing species with finite-rate chemistry. Two temperatures are used to represent translation-rotation energy and vibration energy. The five-species model (N$_2$, O$_2$, NO, N, and O) is used to simulate air. The conservative three-dimensional Navier-Stokes equations consist of five-species mass conservation equations, three momentum conservation equations, the vibration energy conservation equation, and the total energy conservation equation. [10], [11], and [12] have used similar formulations for shock-fitting DNS of thermochemical nonequilibrium flow. Written in vector form the governing equations are

$$\frac{\partial U}{\partial t} + \frac{\partial F_j}{\partial x_j} + \frac{\partial G_j}{\partial x_j} = W \quad (1)$$

where $U$ is the state vector of conserved quantities, and $W$ is the source terms defined by

$$U = \begin{bmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho e \end{bmatrix}, \quad W = \begin{bmatrix} \omega_1 \\ \vdots \\ \omega_{ns} \\ 0 \\ 0 \\ 0 \\ \sum_{s=1}^{nms} (Q_{T-V,s} + \omega_s e_{v,s}) \end{bmatrix}.$$ 

$F_j$ and $G_j$ are the inviscid and viscous fluxes, respectively, and are defined by

$$F_j = \begin{bmatrix} \rho_1 u_j \\ \vdots \\ \rho_{ns} u_j \\ \rho u_1 u_j + p \delta_{1j} \\ \rho u_2 u_j + p \delta_{2j} \\ \rho u_3 u_j + p \delta_{3j} \\ (\rho e + p) u_j \end{bmatrix}, \quad G_j = \begin{bmatrix} \rho_1 v_{1j} \\ \vdots \\ \rho_{ns} v_{nsj} \\ \tau_{1j} \\ \tau_{2j} \\ \tau_{3j} \\ -u_j \tau_{ij} - k_T \frac{\partial T}{\partial x_j} - k_V \frac{\partial T_v}{\partial x_j} + \sum_{s=1}^{nms} \rho_s h_s v_{sj} \\ -k_V \frac{\partial T_v}{\partial x_j} + \sum_{s=1}^{nms} \rho_s e_{v,s} v_{sj} \end{bmatrix}.$$ 

where $v_{sj}$ is the species diffusion velocity, and

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \rho \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (2)$$

is the viscous stress. The total energy per unit volume $\rho e$ is defined by

$$\rho e = \sum_{s=1}^{ns} \rho_s c_{v,s} T + \rho e_v + \frac{1}{2} \rho (u_1^2 + u_2^2 + u_3^2) + \sum_{s=1}^{ns} \rho_s h_s^0 \quad (3)$$

where $h_s^0$ is the heat of formation of species $s$, $e_{v,s}$ is the species specific vibration energy, and $c_{v,s}$ is the species translation-rotation specific heat at constant volume defined as

$$c_{v,s} = \begin{cases} \frac{5}{2} \frac{R}{M_s}, & s = 1, 2, \ldots, nms \\ \frac{3}{2} \frac{R}{M_s}, & s = nms + 1, \ldots, ns \end{cases} \quad (4)$$
The vibration energy per unit volume $\rho_e v$ is defined as

$$\rho_e v = \sum_{s=1}^{\text{ms}} \rho_s e_{v,s} = \sum_{s=1}^{\text{ms}} \rho_s \frac{R}{M_s} \frac{\theta_{v,s}}{\exp \left( \frac{\theta_{v,s}}{T_V} \right) - 1}$$

(5)

where $\theta_{v,s}$ refers to the characteristic temperature of each vibrational mode. The characteristic vibration temperatures are taken from [13].

To model chemical nonequilibrium, three dissociation reactions and three exchange reactions are used. Each reaction is governed by a forward and backward reaction rate determined from

$$k_f = C_f T_d^\alpha e^{-\theta_d/T_a}$$

(6)

$$k_b = k_f / K_{eq}$$

(7)

where all forward reaction rate constants are taken from [13]. The equilibrium coefficient $K_{eq}$ is determined using

$$K_{eq} = A_0 \exp \left( \frac{A_1}{Z} + A_2 + A_3 \ln (Z) + A_4 Z + A_5 Z^2 \right), \quad Z = \frac{10000}{T}$$

(8)

which is a curve fit to experimental data from [13].

To calculate the source term in the vibration energy equation representing the exchange of energy between the translation-rotation and vibration energies the Landau-Teller formulation is used

$$Q_{T-V,s} = \rho_s \left( e_{v,s}(T) - e_{v,s}(T_V) \right) <\tau_s> + \tau_{cs}$$

(9)

where $<\tau_s>$ is the Landau-Teller vibration relaxation time given by [14]. The term $\tau_{cs}$ is from [13] to more accurately model the relaxation time in areas of high temperatures occurring just downstream of the bow shock.

The viscosity of each species is computed using a Blottner curve fit shown in Eq. (10). The coefficients are obtained from [15]. The mixture viscosity is then found using each species viscosity from a mixing rule obtained from [16] (Eq. (11)). The total heat conductivities for each energy mode are computed in a similar fashion as viscosity. The diffusion velocity is calculated using Fick’s law and a constant Schmidt number of 0.5.

$$\mu_s = 0.1 \exp \left[ (A_s^\mu \ln (T) + B_s^\mu) \ln (T) + C_s^\mu \right]$$

(10)

$$\mu = \sum_{s=1}^{\text{ns}} X_s \mu_s / \phi_s$$

(11)

### III. Numerical Method

The numerical method is given for the general curvilinear direct numerical simulation method for a body conforming grid. Then the details of the cut-cell method to treat non-conforming geometries, such as an elliptical surface roughness element, is given.

#### A. DNS Numerical Method

A high-order shock-fitting method developed for perfect gas flow by [17] has been extended for use on thermochemical nonequilibrium flows to compute the flow field between the shock and the body. For shock-fitting computations the shock location is not known a priori, so its position is solved along with the flow field. Since the shock position is not stationary, the grid used to compute the flow field is a function of time. This leads to the coordinate transformation

$$\begin{align*}
\xi &= \xi(x,y,z) \\
\eta &= \eta(x,y,z,t) \\
\zeta &= \zeta(x,y) \\
\tau &= t
\end{align*} \quad \begin{align*}
x &= x(\xi, \eta, \zeta, \tau) \\
y &= y(\xi, \eta, \zeta, \tau) \\
z &= z(\xi, \eta, \zeta, \tau) \\
t &= \tau
\end{align*}$$

(12)
where \( y \) is normal to the body, \( x \) is in the streamwise direction, \( z \) is in the transverse direction, \( \zeta = 0 \), and \( \xi = 0 \). The governing equation can then be transformed into computational space as

\[
\frac{1}{J} \frac{\partial U}{\partial \tau} + \frac{\partial E'}{\partial \xi} + \frac{\partial F'}{\partial \eta} + \frac{\partial G'}{\partial \zeta} + \frac{\partial E'_v}{\partial \xi} + \frac{\partial F'_v}{\partial \eta} + \frac{\partial G'_v}{\partial \zeta} + U \frac{\partial (1/J)}{\partial \tau} = \frac{W}{J}
\]

(13)

where \( J \) is the Jacobian of the coordinate transformation and

\[
E' = \frac{F_1 \xi_x + F_2 \xi_y + F_3 \xi_z}{J}
\]

(14)

\[
F' = \frac{F_1 \eta_x + F_2 \eta_y + F_3 \eta_z}{J}
\]

(15)

\[
G' = \frac{F_1 \zeta_x + F_2 \zeta_y + F_3 \zeta_z}{J}
\]

(16)

\[
E'_v = \frac{G_1 \xi_x + G_2 \xi_y + G_3 \xi_z}{J}
\]

(17)

\[
F'_v = \frac{G_1 \eta_x + G_2 \eta_y + G_3 \eta_z}{J}
\]

(18)

\[
G'_v = \frac{G_1 \zeta_x + G_2 \zeta_y + G_3 \zeta_z}{J}
\]

(19)

A seven point stencil is used to discretize the spatial derivatives

\[
\frac{df}{dx} = \frac{1}{hb_i} \sum_{k=-3}^{3} \alpha_{i+k} f_{i+k} - \frac{\alpha}{6b_i} h^5 \left( \frac{\partial f^6}{\partial \xi^6} \right)
\]

(20)

where

\[
a_{i+3} = \pm 1 + \frac{1}{12} \alpha, \quad a_{i+2} = \pm 9 - \frac{1}{2} \alpha
\]

\[
a_{i+1} = \pm 45 + \frac{5}{4} \alpha, \quad a_{i-1} = - \frac{5}{3} \alpha
\]

\[
b_i = 60
\]

and where \( h \) is the step size, \( \alpha < 0 \) is a fifth order upwind explicit scheme, and \( \alpha = 0 \) reduces to a sixth order central scheme. Here the inviscid terms use \( \alpha = -6 \) which yields a low dissipation fifth order upwind difference and the viscous terms are discretized using \( \alpha = 0 \). The derivatives in the transverse direction—if required—are treated with Fourier collocation. To compute second derivatives, the first order derivative operator is applied twice.

Flux splitting is used for the inviscid flux terms resulting in

\[
F' = F'^+ + F'^-
\]

(21)

where

\[
F'^\pm = \frac{1}{2} (F' \pm \Lambda U)
\]

(22)

and \( \Lambda \) is a diagonal matrix that ensures \( F'^+ \) and \( F'^- \) contain only pure positive and negative eigenvalues, respectively. For thermochemical nonequilibrium, the eigenvalues of \( \Lambda \) were derived in [18].

Conditions behind the shock are calculated from Rankine-Hugoniot relations. In the freestream, the flow is assumed to be in thermal equilibrium and the chemical composition of the flow is frozen. The shock is assumed to be infinitely thin which means that the flow has no time to relax as it crosses the shock as relaxation rates are finite. This leads to the chemical composition remaining constant across the shock, as well as the vibration temperature. Since neither process has any time to relax across the shock, the relaxation zone is entirely downstream of the shock. A complete derivation of thermochemical nonequilibrium shock fitting can be found in [19]. A low storage 3rd-order Runge-Kutta method from [20] is used to advance the solution in time.
B. Cut-Cell Numerical Method

The cut-cell method follows that of [9] and the finite-difference stencils used in the cut-cell method follow that of [21]. A schematic of the cut-cell grid is shown in Fig. 1. The curvilinear grid is only body-fitted to the body which causes the roughness element at the surface of the body to intersect the grid. The curvilinear grid, along with the roughness element, is then transformed from physical space into computational space using the coordinate transform given in Eq. (12). Note that the top of both domains is bounded by the shock and the bottom by the body.

Figure 1. Cut-cell grid in (a) the physical domain and (b) the computational domain from [9].

Once the grid and roughness element have been transformed into computational space, a point classification scheme is required to determine how a given point will be treated. Four different types of grid points are used: regular points, dropped points, irregular points, and boundary points. Figure 2 shows a schematic of point classification in the eta direction. Each of the four point types are shown along with the location of the body overlapping the stencil. Regular points are points in the computational domain where the standard finite difference stencil, given in Eq. (20), is used. That is, there is no infringement of the roughness element onto any of the points used in the standard stencil. The standard stencil here is a centered seven point stencil so three points that are not boundary points are needed to either side of the point for it to be regular. This is shown in Fig. 2 where $\eta_5$ is the first point away from the body that meets this requirement.

There are two types of dropped points. The first type of dropped points are points contained inside of the roughness element. They are denoted by $\bullet$ in Fig. 2. They are not used for any numerical calculations. The second type is points that are deemed too close to boundary points. Locating these dropped points is done in each direction by determining $\sigma$ which is the distance from the point to the body in computational space along a grid line. If $\sigma$ is less than some predefined value, then the point is too close to the body and it is dropped, in that direction, from the finite-difference stencil. Note that, a point may be a dropped point in one grid direction and not in another. A reason for dropping points with a small $\sigma$ is the time step requirement for stability can be severely limited if $\sigma$ is excessively small. Here, $\sigma = 0.5$ is used in each grid.
direction and was found to perform satisfactorily. This choice of \( \sigma \) is made with the implicit assumption that the distance between two points in computational space in any grid direction is unity.

Boundary points are defined as any intersection of a grid line with the roughness element. They are not a part of the original Cartesian grid. At these points, extrapolation of interior flow variables, or their derivatives in the wall normal direction, may be required as boundary conditions. A second-degree least-squares polynomial is used for extrapolation and wall normal derivatives. The polynomial is

\[
f(x, y) = c_1 + c_2 \Delta x + c_3 \Delta y + c_4 \Delta x^2 + c_5 \Delta x \Delta y + c_6 \Delta y^2
\]

where

\[
\Delta x = x - x_{bp}, \quad \Delta y = y - y_{bp}
\]

and where \( f \) is the interpolated variable, the coefficients \( c_1, c_2, \ldots, c_6 \) are found using a least-squares approximation, and the subscript \( bp \) refers to the physical location of the boundary point. The closest twenty one points by index were used to determine the coefficients. This same method was used in [21] where it was found that a least-squares polynomial was more stable than a two-dimensional polynomial interpolation without a least-squares approximation.

Irregular points are points near the roughness element where the standard finite difference grid stencil cannot be used due to an overlap of the stencil with the body. These are points \( \eta_2, \eta_3, \) and \( \eta_4 \) in Fig. 2. Offset stencils, computed from derivatives of Lagrange polynomials, with a non-uniform spacing are used for the irregular points. Here, third-order and fourth-order offset stencils are used for inviscid terms while fourth-order and fifth-order offset stencils are used for the viscous terms. Following the schematic of Fig. 2, a derivative of the upwind flux for the \( j \)th irregular point in computational space is

\[
\frac{\partial F_{j}^{++}}{\partial \eta} = \frac{1}{\Delta \eta} \sum_{k=1}^{6} a_{j,k}^{+} F_{j,k}^{++}.
\]

The coefficients \( a_{j,k}^{+} \) for the inviscid flux terms are given in Table 1 along with the corresponding downwind coefficients. These coefficients are upwind biased. Similarly to Eq. (25), the viscous flux may be found and the corresponding coefficients are given in Table 2. It was shown in [21] that a solution procedure using the coefficients in Tables 1 and 2 along with a fifth-order interior scheme resulted in a fourth order method.

**Table 1. Finite-difference coefficients for inviscid terms at irregular points.**

<table>
<thead>
<tr>
<th>( j )</th>
<th>( a_{j,1}^{+} )</th>
<th>( a_{j,2}^{+} )</th>
<th>( a_{j,3}^{+} )</th>
<th>( a_{j,4}^{+} )</th>
<th>( a_{j,5}^{+} )</th>
<th>( a_{j,6}^{+} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>(- \frac{2}{\sigma (\sigma+1)(\sigma+2)} )</td>
<td>\frac{2-3\sigma}{\sigma}</td>
<td>\frac{2\sigma}{\sigma+1}</td>
<td>\frac{-\sigma}{2(2+\sigma)}</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>\frac{-2}{\sigma (\sigma+1)(\sigma+2)(\sigma+3)}</td>
<td>\frac{2+\sigma}{6\sigma}</td>
<td>\frac{-2-\sigma}{\sigma+1}</td>
<td>\frac{4+\sigma}{2(2+\sigma)}</td>
<td>\frac{2+\sigma}{3(3+\sigma)}</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>\frac{-1}{\sigma (\sigma+1)(\sigma+2)(\sigma+3)}</td>
<td>\frac{-1}{3}</td>
<td>\frac{-1}{3}</td>
<td>\frac{1}{6}</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

**Table 2. Finite-difference coefficients for viscous terms at irregular points.**

<table>
<thead>
<tr>
<th>( j )</th>
<th>( a_{j,1} )</th>
<th>( a_{j,2} )</th>
<th>( a_{j,3} )</th>
<th>( a_{j,4} )</th>
<th>( a_{j,5} )</th>
<th>( a_{j,6} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(- \frac{2(2+\sigma)(\sigma^2+3\sigma+1)}{\sigma(\sigma+1)(\sigma+2)(\sigma+3)} )</td>
<td>\frac{2(\sigma+1)}{2(2+\sigma)}</td>
<td>\frac{-\sigma(\sigma+1)}{2(2+\sigma)}</td>
<td>\frac{\sigma(\sigma+1)}{2(\sigma+3)}</td>
<td>\frac{-\sigma(\sigma+1)}{6(\sigma+3)}</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>\frac{-6}{\sigma(\sigma+1)(\sigma+2)(\sigma+3)}</td>
<td>\frac{-3}{3(\sigma+1)}</td>
<td>\frac{-3}{\sigma+1}</td>
<td>\frac{1}{2(\sigma+2)}</td>
<td>\frac{-\sigma-1}{3(\sigma+3)}</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>\frac{-6}{\sigma(\sigma+1)(\sigma+2)(\sigma+3)}</td>
<td>\frac{-1}{\sigma+1}</td>
<td>\frac{1}{\sigma+1}</td>
<td>\frac{-\sigma-1}{2(\sigma+2)}</td>
<td>\frac{6(\sigma+3)}{3(\sigma+3)}</td>
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</tr>
<tr>
<td>4</td>
<td>\frac{-12}{\sigma(\sigma+1)(\sigma+2)(\sigma+3)(\sigma+4)}</td>
<td>\frac{-2}{3(\sigma+1)}</td>
<td>\frac{-2}{3(\sigma+1)}</td>
<td>\frac{1}{2(\sigma+2)}</td>
<td>\frac{-\sigma-2}{3(\sigma+3)}</td>
<td>\frac{-\sigma-2}{12(\sigma+1)}</td>
</tr>
</tbody>
</table>
IV. Cut-Cell Method Validation

The DNS code for a flow with thermochemical nonequilibrium over a curvilinear grid has been previously validated in [12, 19]. To validate the cut-cell method described in Section III B, two simulations with the same shock-fitting DNS code were run for a flat plate with a single roughness element. The freestream parameters for the case are given in Table 3. Both simulations were run with the same flow parameters and the same roughness element. One simulation used the previously validated curvilinear DNS code with a grid that was body-fitted to the flat plate as well as the roughness. The other simulation used the exact same code except that the grid is only fitted to the flat plate and the roughness element is treated using the cut-cell method. Using these two different simulation techniques makes it so that the main difference between the two simulations is the treatment of the roughness element, thus, testing the newly implemented cut-cell code.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
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<tbody>
<tr>
<td>( M_\infty )</td>
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</tr>
<tr>
<td>( \rho_\infty ) [kg/m(^3)]</td>
<td>( 5.68 \times 10^{-2} )</td>
</tr>
<tr>
<td>( p_\infty ) [N/m(^2)]</td>
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<td>( e_{N_2} )</td>
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<td>( e_{O_2} )</td>
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</tbody>
</table>

A hyperbolic tangent is used for the roughness shape. This shape was chosen because a body-fitted grid may be used and there is a simple analytic form to model the roughness height. Also, the derivatives of the roughness height are continuous which are then used to directly compute the grid metrics for the body-fitted solution. The equation for the roughness height is

\[
 h(x) = \frac{k}{2} \left[ \tanh \left( S_r (x - x_c) + L_r \right) - \tanh \left( S_r (x - x_c) - L_r \right) \right]
\]

where \( k \) is the roughness height at the center line, \( x_c \) is the center of the roughness, \( S_r \) is a shape parameter, and \( L_r \) affects the roughness width. For this test case: \( k = 5 \times 10^{-4} \) m, \( x_c = 0.39 \) m, \( S_r = 3210 \), and \( L_r = 1926 \). These parameters were found to have a negligible effect on the stability of the shock-fitting numerical method when a body-fitted grid was used. This resulted in a more precise comparison between the body-fitted and cut-cell simulations.

The two separate grids for the body-fitted and cut-cell cases are shown in Fig. 3. Only half of the wall-normal points are shown for clarity. Note that the grid for the body-fitted method is more dense near the roughness element when compared to the cut-cell grid. This is due to the wall-normal stretching function that starts at the edge of the roughness element for the body-fitted grid and starts at the flat plate for the cut-cell grid. For this shape, the body-fitted grid is more efficient, but not all roughness shapes can be treated using a body-fitted grid such as an elliptical roughness element which is simulated in Section V.

Both methods were run to solution convergence and then a comparison was performed. A wall-normal velocity contour comparison along with a pressure comparison is given in Figure 4. The solid lines are from the body-fitted solution and the dashed lines are from the cut-cell solution. The roughness height is approximately 7.5% of the velocity boundary-layer thickness with no roughness at \( x = 0.39 \) m. The roughness height was chosen so that there would be no shocks inside the domain as the current implementation of the high-order DNS code only handles shock waves as a boundary of the computational domain. There is little to no visible difference between the two methods near the roughness element. There is some difference in pressure near \( y = 0.002 \) m which is most likely due to the different grid spacing at this location. Overall, the comparison between the two methods is quite good.

Along with contour plots, wall-normal slices were also compared. Fig. 5 shows wall-tangential velocity and temperature profiles at three different streamwise locations. The profiles are located at the center of the roughness (\( x = 0.39 \) m), the upstream curved portion of the roughness (\( x = 0.389 \) m), and the downstream curved portion of the roughness (\( x = 0.391 \) m). The cut-cell solution was interpolated to the body-fitted grid for the comparison. The solutions between the two methods show no visible differences for each of
the profiles. The integrated velocity profiles over the boundary layer showed a 0.25%, 0.16%, and 0.16% difference between the two methods. A percent difference between the two solutions is given for temperature in Figs. 5(d)–5(f). The largest percent difference is located near the edge of the boundary layer and is less than 1%. These results coincide with [21] where solutions between body-fitted and cut-cell methods for a hyperbolic tangent roughness also showed no visible differences.

Overall, the comparison between the body-fitted and the cut-cell solutions is quite good. There is little noticeable difference in wall-normal velocity and pressure contours. The percent difference in temperature profiles at three locations on the roughness is less than 1% for each profile. The cut-cell method accurately compares to the body-fitted method. This information shows that the cut-cell method has been implemented correctly.
Figure 5. Body-fitted and cut-cell solution comparison for (a-c) wall-tangent velocity profiles and (d-f) temperature profiles at select streamwise locations. Body Fitted —, Cut Cell — —, and Percent Difference +.
V. DNS Results of a Flat Plate

To study the effects of roughness on hypersonic boundary-layer instability, multiple direct numerical simulations are run for two separate sets of freestream conditions. Each of these freestream conditions will be covered separately.

Commonly, in studies of boundary-layer instability over a flat plate, a local Reynolds number, \( R \), is used. This Reynolds number is defined as

\[
R = \frac{\rho_\infty u_\infty L}{\mu_\infty}
\]

where \( L \) is the local length scale of the boundary-layer thickness and is defined as

\[
L = \left( \frac{\mu_\infty x}{\rho_\infty u_\infty} \right)^{1/2}.
\]

This local length scale is used here to nondimensionalize the growth rate. The frequency of a boundary-layer mode for LST, or a disturbance simulated in a DNS, is commonly nondimensionalized to obtain

\[
F = \frac{2\pi f \mu_\infty}{\rho_\infty u_\infty^2}
\]

where \( f \) is the dimensional frequency. Also the frequency may be nondimensionalized with a spatial component resulting in

\[
\omega = \frac{2\pi f L}{u} = RF.
\]

Both nondimensionalizations for frequency will be used here.

For a DNS, it is required that the meanflow be perturbed in order to study the growth, or decay, of the perturbation. Here, the flow is perturbed with a suction/blowing slot at the plate surface. The equation for the mass flux of the slot is

\[
\rho v(x,t) w = \epsilon_b (\rho u) \exp \left\{ \frac{-(t-\mu_b)^2}{2\sigma_b^2} \right\} \sin \left\{ \frac{2\pi (x-x_b)}{l_b} \right\}
\]

where \( l_b \) is the length of the slot, \( x_b \) is the center of the slot measured from the leading edge of the flat plate, \( \epsilon_b \) scales the function, \( \mu_b \) shifts the gaussian component to avoid negative times, and \( \sigma_b \) adjusts the spectral content of the function. Notice the time dependent gaussian portion of the function. When transformed to frequency space, this yields a continuous range of frequencies with non-zero amplitudes making this particular approach for perturbing the meanflow an effective strategy when studying a wide range of frequencies.

A. DNS Results for M=10 Flat Plate

The first set of freestream conditions are from the previous LST studies of [22] and [23] that investigated second-mode instability of a real-gas flow over a flat plate. The freestream conditions are given in Table 3. The freestream unit Reynolds number, \( Re_u \), is \( 10.9 \times 10^6 \) /m and the freestream stagnation enthalpy, \( h_{\infty,\infty} \), is 5.9 MJ/kg.

A schematic of the DNS simulation is given in Fig. 6. The inlet, outlet, shock, roughness element, and blowing/suction slot are noted on the figure along with the flat plate which is located at \( y = 0 \). The computational domain is bounded by the inlet, outlet, shock, and flat plate. For the DNS simulation, the meanflow is initially converged to a specified tolerance. This tolerance must be below the linear forcing of the blowing/suction slot or numerical noise will contaminate the unsteady results. Next, the slot is activated, and a linear perturbation is introduced at the slot. This perturbation is then simulated as it travels throughout the meanflow.

In order to quantify roughness effects on the instability process, multiple cases are run for varying roughness heights. These cases are defined in Table 4 which shows that case 1 has no roughness element, while cases 2 and 3 have a roughness element of the same width but different height. Only the roughness height is varied as it was shown in [6] that varying the roughness height plays a much more significant role in
second mode suppression than varying the width. The roughness elements have an elliptical shape defined by

\[
\frac{(x - x_c)^2}{a^2} + \frac{y^2}{h^2} = 1 \tag{32}
\]

where \(x_c\) is the center of the roughness element and \(2a\) is the width. For this case, \(x_c = 0.27\) m and \(a = 2.55 \times 10^{-3}\) m.

Table 4. Case numbers for \(M=10\) flat plate DNSs.

<table>
<thead>
<tr>
<th>Case Number</th>
<th>(h/\delta)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>25.0%</td>
</tr>
<tr>
<td>3</td>
<td>37.5%</td>
</tr>
</tbody>
</table>

Before analyzing the simulation results, a grid convergence study was performed to ensure that the computational grid was sufficiently dense to capture the relevant flow physics. The first grid used 642 by 241 points in the streamwise and wall-normal directions, respectively. The second grid was a double grid solution which used 1282 by 481 points. Case 2 was used as the test case for the grid convergence study. For both grids, the meanflow solution was converged within a specified tolerance and then a perturbation was simulated. Figure 7 shows the frequency spectrum of the wall-pressure perturbation directly behind the roughness at \(x = 0.28\) m. There are only minimal differences between the two simulations. The lack of any significant difference between the two separate results shows that the single grid result is grid converged.

Figure 7. Comparison of single grid (642 by 241) results to double grid (1282 by 481) results for case 2. single grid \(\cdash\), double grid \(\cdash\).
1. Steady Flow Simulations for \( M=10 \) Flat Plate

The first part of the direct numerical simulation is to simulate the time invariant meanflow. Figure 8 shows the meanflow pressure contours for cases 2 and 3. Initially, the roughness element compresses the incoming flow which is shown by the increase in pressure near \( x = 0.26 \) m to the center of the roughness element. This compression turns into a Mach wave which travels downstream. As the roughness height is increased, the strength of this Mach wave increases and will eventually become a shock wave. After this compression, there is a flow expansion on the leeward side of the roughness element resulting in a decreased pressure. Also, it can be seen that as the height of the roughness element is increased, its effects are present further upstream.

![Figure 8. Meanflow solutions of pressure for (a) case 2 and (b) case 3.](image)

Meanflow simulations are also shown in Fig. 9 for the translation-rotation temperature and \( 1 - T/T_V \) near the roughness element for cases 1 and 3. For case 1, the translation-rotation temperature contour remains nearly constant in the streamwise direction over the region shown. Similarly, contours of \( 1 - T/T_V \) remain constant in the streamwise direction over the region shown. For case 3, there is a noticeable increase in translation-rotation temperature as the flow reaches the bump due to the flow compression. After the bump, the flow expands and the temperature decreases. The maximum translation-rotation temperature at \( x = 0.28 \) m for case 3 is actually 20 K less than the maximum value for case 1. As the flow moves further downstream, the maximum temperature for case 3 approaches the value of case 1.

2. Unsteady Flow Simulations for \( M=10 \) Flat Plate

Figure 10 shows the wall-normal mass flux imposed at the centerline \((x = x_b)\) of the surface blowing/suction slot. For cases 1–3, \( x_b = 0.15 \) m \(( R(x_b) = 1719)\), \( l_b = 0.002 \) m, \( \epsilon_b = 1 \times 10^{-4} \), \( \mu_b = 3 \times 10^{-6} \), and \( \sigma_b = 8 \times 10^{-7} \). These parameters were chosen to ensure that the perturbation is linear, as well as ensuring larger forcing amplitudes for the frequencies of interest. As the gaussian function has tails that approach zero at infinity, the function needs to be truncated while not strongly affecting the frequency content. Here, the function was truncated at \( t = 6 \times 10^{-6} \) s without any adverse effects. Figure 10(b) shows the analytic Fourier transform, along with the discrete Fourier transform (DFT) obtained from the DNS results, at \( x = x_b \). The two results lie directly on top of one another, as they should. Note that most of the spectral energy density is contained in the range \( 0 \leq f \leq 400 \) kHz. This was done to strongly force the frequencies near the second mode.

Before analyzing the unsteady results, a comparison with previous findings for the same flow conditions is performed to show that the current findings are consistent with previous results. A comparison of the growth rate and phase velocity of the second mode to the previous results of [23] is shown in Fig. 11. In [23], the same thermochemical nonequilibrium model is used for solution of the meanflow except the reactions and reaction rates differ. Overall the growth rate compares quite well. The maximum amplification, as well as the frequency at maximum amplification, compare well. There is some difference in the phase velocity for \( \omega > 0.7 \) and the reason for the small difference is unclear. Likely it is due to the differences in the gas.
Figure 9. Steady state solutions of (a–b) translation-rotation temperature and (c–d) $1 - T/T_V$.

Figure 10. The (a) mass flux imposed at $x = x_b$ and (b) comparison of the Fourier transform to the discrete Fourier transform obtained from DNS.

Figure 11. Comparison at $R = 739.6$ of (a) growth rate and (b) phase velocity to [23]. Current work $\rightarrow$, and [23] $\bullet$. 
model or perhaps small differences in the meanflow. Overall, the comparison between the two methods is adequate, showing that the current results follow previous findings.

When the blowing/suction slot is activated in a DNS, the disturbance is not a pure mode. As the disturbance travels downstream, some frequency components will grow and some will decay. Further, each frequency component can be composed of multiple modes that may individually grow or decay. As one mode begins to dominate for a single frequency component, i.e., its amplitude grows much larger than any other mode’s amplitude, it is possible to achieve an accurate comparison for that mode between a DNS and LST calculations. Figure 12 shows a comparison of the growth rate and phase velocity obtained from a DNS to those obtained from LST for case 1. Near the blowing/suction slot ($R = 1719$), the DNS results do not match either mode F or mode S. However, near $R = 1900$, the DNS results match closely with mode S, or the second mode, predicted by LST. This shows that as the disturbance travels downstream, the second mode begins to grow significantly and dominate the other boundary-layer modes at that frequency. Also, this shows that the disturbance created by the blowing/suction slot is developing into the second mode.

![Figure 12. Comparison of DNS ( ) at $F = 4.28 \times 10^{-5}$ for case 1 with mode S ( ) and mode F ( ) obtained from LST.](image)

In the previous results of [3, 4, 5, 6], it was found that for a fixed frequency, when a roughness element was placed upstream of the synchronization point in a hypersonic boundary layer, the second mode was destabilized. Conversely, when it was placed downstream of the synchronization point, the second mode was stabilized. It should be noted that the synchronization point referred to is obtained from the meanflow solution without any surface roughness. Here, that would refer to case 1. Therefore, for analysis of the DNS results, it is necessary to find the synchronization point of mode S and mode F using LST from the meanflow of case 1. Figure 13 shows the phase velocity and growth rate for mode S and mode F at $R=1719$. Recall that the roughness is located at $R=1719$. This figure is obtained by fixing the streamwise location and varying the frequency. To differentiate between the first discrete mode that originates from the fast acoustic spectrum and the second, the terminology “mode F I” is used to refer to the first and “mode F II” used for the second. Mode F I synchronizes with mode S at $\omega = 0.085$, or $F = 4.94 \times 10^{-5}$. Therefore, it is expected that frequencies above $F = 4.94 \times 10^{-5}$ will be damped while frequencies below $F = 4.94 \times 10^{-5}$ will be amplified.

Figure 14 shows the wall-pressure perturbation for two fixed frequencies. The break in the lines of each plot for cases 2 and 3 is due to the surface roughness. The first frequency, $F = 3.43 \times 10^{-5}$, is below the frequency at the synchronization location so it is expected that it will be amplified compared to case 1. Each of the three cases start with the same pressure perturbation near $R = 1600$. As the perturbation approaches the roughness element, the wall-pressure perturbation increases wildly. After the roughness, there is some slight damping before the wall-pressure perturbation grows again and becomes larger than the perturbation for case 1. This growth is second mode growth. Recall from Fig. 13 that the growth in the DNS disturbance was similar to LST predictions of the growth rate and phase velocity of the second mode. Also note that, as the roughness height increases, the growth of the disturbance increases. These findings that a frequency below the synchronization frequency is amplified, and a larger roughness height more strongly amplifies the second mode, correspond with the previous results of [3, 4, 5, 6].
The second frequency, $F = 5.14 \times 10^{-5}$, is above the frequency at the synchronization location so it is expected that it will be damped when compared to case 1. Each of the three cases start with the same pressure perturbation near $R = 1600$. Similar to $F = 3.43 \times 10^{-5}$, as the perturbation approaches the roughness element, the wall-pressure perturbation increases wildly. After the roughness element, the wall-pressure perturbation stays damped for the remaining portion of the simulation. Also, as the roughness height is increased, the corresponding damping of the wall-pressure perturbation is decreased. These findings that a disturbance at a frequency below the synchronization frequency is damped, and a larger roughness height more strongly damps the second mode, correspond with the previous results of [3, 4, 5, 6].

Similar to analyzing a single frequency along the flat plate, since the frequency content of the perturbation is continuous, it is possible to fix the streamwise location and visualize the frequency spectra. Figure 15 shows the wall-pressure perturbation spectra at two separate streamwise locations. The large amplitudes are due to the growth of the second-mode instability. The first location, $R = 1687$ is upstream of the roughness element. Notice that for both roughness cases the perturbation is amplified for almost the entire frequency range. Upstream of the roughness, the effects of the roughness are to amplify each frequency component. The second location, $R = 1985$, is downstream of the roughness element. Now the damping effect due to the roughness element is clear. The amplifying effect of the roughness on the second mode is slight at this streamwise location but still visible for case 3 at $F = 5 \times 10^{-5}$. 

Figure 13. Plot of (a) phase velocity and (b) growth rate at the fixed location $R = 1719$.

Figure 14. Wall-pressure perturbation for cases 1–3 of a single frequency (a) below and (b) above the synchronization frequency.
Figure 15. Wall-pressure perturbation frequency spectra for cases 1–3 at a location (a) upstream and (b) downstream of the roughness element.

Overall, the results for the Mach 10 flat plate cases 1–3 of a real-gas flow were shown to be consistent with previous research for hypersonic flows with a perfect gas assumption. It was shown that a two-dimensional roughness element can suppress second-mode instability in a real gas. These results show that the idea of stabilizing a hypersonic boundary layer through use of two-dimensional roughness elements does extend to real gas flows.

B. DNS Results for M=15 Flat Plate

The second set of freestream conditions are also from the previous LST studies of [22] and [23] for second-mode instability of a real-gas flow over a flat plate. They are given in Table 5. The freestream unit Reynolds number, \( Re_u \), is \( 3.33 \times 10^6 \) /m and the freestream stagnation enthalpy, \( h_{o,\infty} \), is 32.6 MJ/kg. The boundary conditions at the flat plate are no-slip for each of the velocities, a constant wall temperature of \( T_w = T_{V,w} = 1225 \) K, and non-catalytic conditions for each of the chemical constituents.

Table 5. Freestream conditions for Mach 15 flat plate.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M_\infty )</td>
<td>15.0</td>
</tr>
<tr>
<td>( \rho_\infty ) [kg/m(^3)]</td>
<td>( 1.391 \times 10^{-2} )</td>
</tr>
<tr>
<td>( p_\infty ) [N/m(^2)]</td>
<td>2812</td>
</tr>
<tr>
<td>( c_{N_2} )</td>
<td>0.78</td>
</tr>
<tr>
<td>( c_{O_2} )</td>
<td>0.22</td>
</tr>
</tbody>
</table>

In an attempt to quantify real gas and roughness effects in the instability process, multiple cases are run for varying gas models and roughness heights. These cases are defined in Table 6. The cases are a mix of varying roughness heights and either a real gas, or a perfect gas, model. The perfect gas model is obtained from the real gas model described in Section II. For the case of a perfect gas, the source terms are turned off, the vibration energy is held constant, and the mass fractions are held to their freestream values. This is done so that the viscosity, thermal conductivity, etc., are calculated the exact same way for either the real, or perfect, gas.

Before analyzing the simulation results, a grid convergence study was performed to ensure that the computational grid was sufficiently dense to capture the relevant flow physics. The first grid used 962 by 241 points in the streamwise and wall-normal directions, respectively. The second grid was a double grid solution which used 1922 by 481 points. Case 5 was used as the test case for the grid convergence study. For both grids, the meanflow solution was converged within a specified tolerance and then a perturbation was
simulated. Figure 16 shows the frequency spectra of the wall-pressure perturbation over the region tested. There are only minimal differences between the two simulations. The lack of any significant difference between the two separate results shows that the single grid result is grid converged.

1. Steady Flow Simulations for M=15 Flat Plate

The first step in the direct numerical simulation is to simulate the time invariant meanflow. Figure 17 shows the meanflow contours of the translation-rotation temperature and $1 - T/T_V$ near the roughness element for cases 4 and 7. For case 4, the translation-rotation temperature contour remains nearly constant in the streamwise direction over the region shown. However, the vibration temperature is increasing and equilibrating with the translation-rotation temperature as the flow moves downstream. For case 7, the roughness element compresses the flow and causes a strong increase in translation-rotation temperature near $0.185 \text{ m} \leq x \leq 0.19 \text{ m}$. Behind the roughness, the maximum translation-rotation temperature is higher than case 4. Also, the vibration temperature is increased and moves closer to equilibrium with the translation-rotation temperature behind the roughness element. Overall, the roughness element serves to increase the translation-rotation temperature of the flow and move the vibration temperature closer to thermal equilibrium.
Figure 17. Meanflow contours of translation-rotation temperature for (a) case 4 and (b) case 7 along with contours of $1 - T/T_V$ for (c) case 4 and (d) case 7.

Figure 18 shows the meanflow contours of temperature for cases 8 and 11. Similar to the roughness element in a real gas flow, the roughness element in the perfect gas flow increases the temperature immediately upstream of the roughness. It also increases the maximum temperature in the boundary layer downstream of the roughness in the range $x \geq 0.2$ m. Overall, the temperature for the perfect gas flow is higher than that for a real gas. This makes sense as energy is input into chemical reactions, as well as higher energy modes, for the real gas flow which are not present in the perfect gas flow.

Figure 18. Meanflow contours of the temperature for (a) case 8 and (b) case 11.

Figure 19 gives a comparison of cases 4 and 7 with cases 8 and 11 at two separate streamwise locations. The first location—$x = 0.22$ m (R=856.0)—is 19.6δ downstream of the roughness element. Both temperatures have clearly increased for case 7 compared to case 4 with the maximum vibration temperature increasing nearly 600 K. Similarly, the temperature for case 11 has clearly increased when compared to case 8. The second location—$x = 0.37$ m (R=1110)—is 117.6δ downstream of the roughness element. The difference between the temperatures here is much less pronounced. Near the wall, there is little distinguishable difference between any of the profiles. There is some difference in the translation-rotation temperature for cases 4 and 7 where $y > 0.003$ m due mainly to boundary-layer thickening. For the vibration temperature, there is still an increase in the maximum value but it is not as pronounced as before. For cases 8 and 11, there is also an increase in the maximum value, but again, it is not as pronounced as before. Overall, as the flow moves downstream, the roughness perturbed meanflow approaches the unperturbed meanflow with a slight shift due to boundary-layer thickening.
Figure 19. Wall-normal profiles of temperatures at (a) $x = 0.22$ m ($R = 856.0$) and (b) $x = 0.37$ m ($R = 1110$).

As the roughness element strongly increases the translation-rotation temperature, it is expected that this will have an effect on the chemical composition of the flow. The reaction this increase in temperature is likely to affect the most is the dissociation of oxygen. Figure 20 shows the contours of the mass fraction of atomic oxygen for cases 4 and 7. There is an increase in $c_O$ for case 4 in the downstream direction, as well as for case 7. However, the increase in $c_O$ for case 7 is much larger due to the increased temperatures created by the roughness element. As $c_O$ increases, the flow moves closer to chemical equilibrium.

![Figure 20. Meanflow contours of the mass fraction of atomic oxygen.](image)

To compare the concentration of $c_O$ between cases 4–7, Fig. 21 shows the wall-normal profiles of the mass fraction of atomic oxygen at two separate streamwise locations. For each case the roughness element increases the concentration of atomic oxygen with the largest roughness case creating the highest concentration of atomic oxygen. As the flow moves far downstream from the roughness element to $x = 0.37$ m, the concentration of atomic oxygen is still significantly larger for case 7 than case 4. This is unlike the temperatures which are approaching the same value.

A common question that naturally arises when studying the flow over a perturbed surface is, “how does the perturbation affect the surface heat transfer?” If the surface heat transfer induced by the perturbation is larger than the heat transfer obtained from a turbulent flow, then the purpose of delaying transition by judiciously placed surface roughness is partially defeated. Figure 22(a) shows the wall heat flux from case 2 with and without surface roughness. The two results begin to diverge near $R = 770$ where the roughness case actually has less heat transferred to the wall than the clean case. At the roughness, the wall heat flux for the roughness case is nearly 5 times larger than the clean case. However, this rise in heat flux is only over a small portion of the plate. Downstream of $R = 900$, the heat flux for the clean and roughness cases converges to the same value.

Clearly, there is a difference in the local surface heat flux near the element, but how does this affect the total energy transferred to the vehicle surface? In Fig. 22(a), the total heat transferred to the vehicle is shown. The total heat transfer is obtained by integrating, along the body surface, the local surface heat flux.
Figure 21. Wall-normal profiles of the mass fraction of atomic oxygen at (a) \( x = 0.22 \) m \( (R = 856.0) \) and (b) \( x = 0.37 \) m \( (R = 1110) \).

Figure 22. Comparison of (a) wall heat flux and (b) total wall heat transfer for cases 4 and 7. Roughness at \( R = 795.5 \). Case 4 - - - , Case 7 ----.

As the flat plate is infinite in the transverse direction, the result is given in units of power over length. It can be seen that the difference between the clean and perturbed surface is small. At \( R = 1000 \), the difference between the two is 0.04%. This small difference shows that, for a single roughness element, there is no significant change in the total heat transferred to the vehicle surface. To summarize, near the roughness there are strong local variations in the surface heat flux, however, the total heat transferred to the surface remains relatively unaffected when a single roughness element is added to the flat plate’s surface.

2. Unsteady Flow Simulations for \( M=15 \) Flat Plate

Figure 23 shows the wall-normal mass flux imposed at the centerline \((x = x_b)\) of the surface blowing/suction slot. For cases 4–11, \( x_b = 0.10 \) m, \( l_b = 0.002 \) m, \( \epsilon_b = 1 \times 10^{-6} \), \( \mu_b = 3 \times 10^{-6} \), and \( \sigma_b = 5 \times 10^{-7} \). These parameters were chosen to ensure that the perturbation is linear, as well as ensuring larger forcing amplitudes for the frequencies of interest. As the gaussian function has tails that approach zero at infinity, the function needs to be truncated while not strongly affecting the frequency content. Here, the function was truncated at \( t = 6 \times 10^{-6} \) s without any adverse effects. Figure 23(b) shows the analytic Fourier transform, along with the discrete Fourier transform (DFT) obtained from the DNS results, at \( x = x_b \). The two results lie directly
on top of one another, as they should. Note that most of the spectral energy density is contained in the range $0 \leq f \leq 700 \text{ kHz}$. This was done to strongly force the frequencies near the second and third modes.

Before analyzing the unsteady results, a comparison with previous findings for the same flow conditions is performed to show that the current findings are consistent with previous results. A comparison of the growth rate and phase velocity of the second mode to the previous results of [22] is shown in Fig. 24. In [22], a boundary layer solver is used to compute the meanflow which is modeled using an assumption of chemical equilibrium. This differs from the thermochemical nonequilibrium assumption used here and the shock-fitting method used to simulate the meanflow. Considering the differences, the two results match quite well. The maximum amplification, as well as the frequency at maximum amplification, compare well. There is some difference in the amplification rate near $0.06 < \omega < 0.08$. However, this difference could be due to the different gas models used, or, the solution procedure of the meanflow. Similarly, the phase velocity compares well over the region of second mode instability. Away from the second-mode unstable region, near the tails of the plot, the differences are larger. Overall, considering the two different gas models and solution procedures, the comparison between the two methods compares quite well showing that the current results match well with previous findings.

Instantaneous snapshots of the translation-rotation and vibration temperatures for cases 4 and 7 are shown in Fig. 25. In Figs. 25(a) and 25(b) there is a Mach wave visible near $y = 0.001 \text{ m}$. This Mach wave is due to the flow adjusting to the initial perturbation at the wall. It is about an order of magnitude larger.
than any other flow disturbance. The Mach wave is not visible in the vibration temperature plots because the induced perturbation from the Mach wave is too weak. Also, notice that the original Gaussian forcing has changed to a pattern that is clearly oscillatory. As the initial disturbance enters the boundary layer, it excites boundary-layer modes for different frequencies that grow and/or decay at different rates. These boundary-layer modes are oscillatory in nature thus creating the oscillatory structure in the figures.

Figure 25. Instantaneous translation-rotation temperature and vibration temperature perturbation from DNS.

Between the Mach wave and the wall, the largest perturbation amplitudes are found near the leading edge of the perturbation near $x = 0.2$ m. Moving upstream, the perturbation gradually decreases until it reaches far enough upstream where it decays to zero. Both temperatures have an oscillation in amplitude near the boundary-layer edge and the wall. The oscillation near the wall is much stronger for translation-rotation temperature than vibration temperature. These oscillations are characteristic of a second-mode wave in a hypersonic boundary-layer where the translation-rotation temperature eigenfunction has large amplitudes near the boundary-layer edge and wall. For Figs. 25(a) and 25(c), the oscillatory pattern is smooth and continuous. However, when the roughness is added to the meanflow as shown in Figs. 25(b) and 25(d), this pattern is adjusted. From $0.18 \leq x \leq 0.19$ m, there is a squishing together of the high and low amplitudes as the disturbance moves into the compression region in front of the roughness element. Behind the element in the region $0.19 \leq x \leq 0.20$ m, the low amplitude disturbance at the wall is stretched out and decreased in magnitude when compared to the flow with no roughness. Also, the high amplitude disturbance is pushed away from the wall.

An instantaneous snapshot of the pressure perturbation is given in Fig. 26. Similar to the perturbation of translation-rotation temperature, there is a Mach wave near $y = 0.001$ m due to the flow adjusting to the initial gaussian forcing. Towards the wall, the pressure perturbation is characteristic of a second-mode wave in a hypersonic boundary-layer with the largest amplitude found at the wall. Again, before the roughness, the disturbance seems to squash together where behind the roughness it seems to stretch out. Note how downstream of the roughness there are two more peaks in pressure where upstream of the roughness there is only one. This is due to the fact that after the roughness the pressure disturbance is traveling along the compression and expansion waves present in the meanflow.

In order to determine the synchronization location of the fast (mode F) and slow (mode S) acoustic modes, the phase velocity and the growth rate of the modes were computed using LST and are shown in Fig. 27. This plot is found using the meanflow of case 4 and fixing the location while varying the frequency. The location corresponds to the center of the roughness element at $x=0.19$ m which corresponds to $R=795.5$. The synchronization location of mode F and mode S is loosely defined as the location where the phase velocities of the modes are equal rather than the more strict definition requiring both the real and imaginary parts of
\( \alpha \) to be equal. This occurs at \( \omega = 0.056 \) which corresponds to \( F = 7.06 \times 10^{-5} \). Although it is not shown, the perfect gas synchronization frequency was found to be \( \omega = 0.055 \) which corresponds to \( F = 6.96 \times 10^{-5} \). Similarly, the synchronization location between mode S and the second discrete mode originating out of the fast acoustic spectrum (mode F II) can be found. This synchronization occurs at \( \omega = 0.128 \) which corresponds to \( F = 1.615 \times 10^{-4} \). There is no change in the synchronization frequency for the third mode in the perfect gas flow.

Figure 28 shows contour plots of wall-pressure perturbation for cases 4–7. These figures show the frequency range over which the second mode is unstable. Note that the roughness element for cases 5–7 is located at \( R = 795.5 \). For case 4 where there is no roughness element, the contours are smooth and ordered. There is a clear high amplitude region running across the figure from \( F = 9 \times 10^{-5} \) at \( R = 750 \) to \( F = 7 \times 10^{-5} \) at \( R = 1100 \). This high amplitude region is caused by second-mode growth. For the cases with roughness elements, the contours are less ordered and the clear region of second-mode growth changes. For each roughness case, there are wild oscillations in amplitude immediately upstream of the roughness element. These oscillations are not dependent on the frequency, rather each frequency experiences them. Near the region of second mode growth, these wild oscillations can lead to large amplitudes before the roughness element. However, behind the roughness element these oscillations are quickly damped. As the roughness element increases in height, the clearly defined second mode region in Fig. 28(a) slowly changes until in Fig. 28(d) where the second mode region looks like it is almost split into two separate horizontal sections. The frequency at which this splitting occurs corresponds roughly to the synchronization frequency which was found to be \( F = 7.06 \times 10^{-5} \).

Figure 29 shows contour plots of wall-pressure perturbation over the third-mode frequency range for cases 4–7. These figures show the frequency range over which the third mode is unstable. Note that the roughness element for cases 5–7 is located at \( R = 795.5 \). For case 4 where there is no roughness element, the
Figure 28. Contour plots of wall-pressure perturbation for the second mode.

Contours are more smooth and ordered. There is a clear high amplitude region running across the figure from $F = 1.8 \times 10^{-4}$ at $R = 750$ to $F = 1.2 \times 10^{-4}$ at $R = 1100$. This high amplitude region is caused by third-mode growth. The waviness seen in the contours of Fig. 29(a) for frequencies higher than $F = 1.8 \times 10^{-4}$ is due to modulation caused by multiple boundary layer modes all present in the boundary layer simultaneously. For the cases with roughness elements, the contours are less ordered and the clear region of third-mode growth changes. For each roughness case, there are wild oscillations in amplitude immediately upstream of the roughness element. These oscillations are not dependent on the frequency, rather each frequency experiences them. Near the region of third-mode growth, these wild oscillations can lead to large amplitudes before the roughness element. However, behind the roughness element these oscillations are quickly damped. As the roughness element increases in height, the clearly defined third-mode region in Fig. 29(a) slowly changes until in Fig. 28(d) where the third-mode region looks like it is almost split into two separate horizontal sections. The frequency at which this splitting occurs corresponds roughly to the synchronization frequency of mode S and mode F II which was found to be $F = 1.615 \times 10^{-4}$.

Figure 30 shows the wall-pressure perturbation contours for cases 8 and 11. These are the ideal gas cases that correspond to the real gas cases 4 and 7. Qualitatively, the contour plots of the wall-pressure
perturbation for the second mode are the same for each of the ideal gas cases. However, the amplitude for the ideal gas cases is slightly lower. Similarly, the contour plots of the wall-pressure perturbation for the third mode are the same for the ideal gas. However, there is no noticeable decrease in the amplitude of the third mode.

To analyze which frequencies are stabilized and/or destabilized by the roughness elements, Fig. 31 shows the wall-pressure perturbation for cases 4–7 of a single frequency below and above the synchronization frequency. The frequency below the synchronization frequency is destabilized for each of the cases with a roughness element when compared to the case without a roughness element. This destabilizing effect is rather small but it is noticeable. Also, the destabilizing effects increase as the roughness height increases. Conversely, the frequency above the synchronization frequency is stabilized for each of the cases with a roughness element. This stabilizing effect is rather weak for cases 5 and 6 and is much stronger for case 7. Clearly, for this frequency, the resultant damping due to changing the roughness height is nonlinear. This is unlike the destabilizing effect shown in Fig. 31(a) where the resultant growth due to changing the roughness height is close to linear. These effects are most likely associated with the roughness height rather than the gas model as the perfect gas simulations show the exact same behavior.
Figure 32 shows the wall-pressure perturbation spectra near the frequency range of the second and third modes. The growth in the wall-pressure perturbation in Fig. 32(a) is due to the second mode and the growth in Fig. 32(b) is due to the third mode. From Fig. 32(a), it is seen that as the roughness height increases, the amplitude of the perturbation decreases and moves to a lower frequency. Also, similar to the single frequency results of Fig. 31(a), the decrease in amplitude is nonlinear. For Fig. 32(b), the results are less clear. While it seems that the roughness elements are damping the third mode, the damping is not as large as the second mode. Part of this is due to the fact that the growth rate of the third mode is about one third of the second mode’s growth rate. With this small of a growth rate, the third mode is not clearly the dominant instability mode over this frequency range. This is shown by the waviness in the wall-pressure perturbation. This waviness is not seen in Fig. 32(a) over the second mode frequency range.

The difference between the perfect gas and real gas cases at the frequencies $F = 4.73 \times 10^{-5}$ and $F = 7.09 \times 10^{-5}$ for the wall-pressure perturbation is shown in Fig. 33. It is interesting to note that either with or without a roughness element the ideal gas case has a larger amplitude at $R = 1100$ for $F = 4.73 \times 10^{-5}$. This is likely caused by the slightly thicker boundary layer for the perfect gas which causes the second-mode instability to move to a lower frequency range. However, this difference is minimal and the two gas models
behave almost identically. For $F = 7.09 \times 10^{-5}$, the real gas perturbation is larger over the entire domain either with or without roughness.

Figure 34 shows a comparison of cases 4, 7, 8, and 11 at $R = 948$ for the second and third modes. The difference between cases 4 and 8, as well as the difference between cases 7 and 11, is the gas model. The difference between cases 4 and 7, as well as cases 8 and 11, is the roughness height. The percent difference of the maximum amplitude between cases 4 and 7 in Fig. 34(a) for the second mode is 40.0%. The percent difference of the maximum amplitude for the second mode between cases 8 and 11 is 34.9%. These differences are due solely to the damping effect of the roughness. Taking this information into account, it follows that the real-gas flow with a roughness element at $R = 948$ is damping the maximum second-mode instability 5.1% more than the corresponding perfect-gas flow. In other words, the real gas with roughness flow is more effective at damping the maximum second-mode instability than the corresponding perfect gas flow. There are a couple of possible explanations as to why the roughness element more effectively damps the
Figure 33. Comparison of the wall-pressure perturbation at two distinct frequencies.

Figure 34. Comparison of the wall-pressure perturbation at $R = 948$ for cases 4, 7, 8, and 11 for (a) the second mode and (b) the third mode.
second mode instability in the real-gas flow. Recall from Fig. 19(a) that the roughness element for case 7 significantly increases the vibration temperature moving it closer to equilibrium with the translation-rotation temperature. Also, recall from Fig. 20 that these increases in temperature cause oxygen in the real-gas flow to dissociate and form a larger amount of atomic oxygen. Both of these physical phenomena require a closer look to determine exactly what is responsible for the increased damping.

For the third mode region shown in Fig. 34(b), the results are different than the second mode. Both of the gas models damp the third mode the same amount and the stronger real gas stabilizing effects are not seen. The reasons for this are currently unclear. The third-mode instability may not be large enough to dominate other boundary-layer modes at the same frequency making the damping effects on only the third mode unclear. Also, it is possible that the third mode damping by surface roughness is truly unaffected by the gas model. Further study must be done to determine the cause.

VI. Conclusions

The objectives of this paper are 1) to validate a new high-order shock-fitting direct simulation method for hypersonic flows with thermochemical nonequilibrium and arbitrary surface roughness, and 2) to study, by DNS, the effects of two-dimensional roughness elements in a real-gas flow on hypersonic boundary-layer instability over a flat plate. A set of five species is used to model chemical nonequilibrium where a two-temperature model is used for thermal nonequilibrium. A cut-cell method is used to simulate arbitrary shaped surface roughness elements that cannot be simulated with a body conforming grid.

The method validation is performed with a geometry that may be simulated with a body-fitted grid or a cut-cell grid. There is little noticeable difference in wall-normal velocity and pressure contours between the two grid solutions. The percent difference in temperature profiles at three separate streamwise locations is less than 1% for each profile. Overall, the simulation of the flow on the cut-cell grid accurately compared to the simulation performed on the body-fitted grid showing that the implementation of the cut-cell method is valid.

Two separate meanflow conditions were used to study hypersonic boundary-layer instability in a real gas over a flat plate. For a Mach 10 flow, it was found that a roughness element placed downstream of the synchronization location of mode S and mode F stabilized the second mode. When the same roughness element was upstream of the synchronization location for a given frequency, the second mode was destabilized. These results are consistent with the results of previous researchers for a perfect gas.

For a Mach 15 flow, both real-gas and perfect-gas simulations were run with and without surface roughness. The real-gas flow with a roughness element resulted in a 40.0% reduction in the maximum amplitude of the second mode where the perfect-gas flow with a roughness element resulted in a 34.9% reduction. The real-gas flow with a two-dimensional roughness element more effectively stabilized the second-mode instability when compared to a perfect-gas flow. Also, the third mode was found to be moderately stabilized by a roughness element for both a real-gas and perfect-gas flow. The stronger stabilizing effect for a real gas was not visible for the third mode, rather both gas models stabilized the third mode the same amount.

VII. Future Work

To further understand how two-dimensional surface roughness elements affect second-mode instability in a real-gas hypersonic boundary layer, it would be useful to use the new method described here to simulate a blunt geometry where real gas effects are, in general, stronger. Specifically, it would be useful to use the Mach 10 flow conditions described here to study the flow over a blunted plate. The blunted plate should significantly alter the chemical composition of the flow, as compared to a perfect gas, hopefully revealing a more complete understanding of the effects on second-mode instability for a two-dimensional roughness element in a real-gas boundary layer.

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