

To the Graduate Council:

I am submitting herewith a dissertation written by Ethan Vogel entitled "Entropy-Based Analysis for Application to Highly Compressible Flows." I have examined the final paper copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Aerospace Engineering.

Dr. James Coder, Major Professor

We have read this dissertation
and recommend its acceptance:

Damiano Baccarella

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(Original signatures are on file with official student records.)

Entropy-Based Analysis for Application to Highly Compressible Flows

A Dissertation Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Ethan Vogel
December 2021

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*To my wonderful wife Jenna, who has received far more thermodynamics lectures
than any veterinarian should have to.*

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No structure, even an artificial one, enjoys the process of entropy. It is the ultimate fate of everything, and everything resists it.

-Philip K. Dick

Abstract

Matrix normalizations are a critical component of mathematically rigorous aerodynamics analysis, especially where kinematic and thermodynamic behaviors are of interest. Here, a matrix normalization based around the entropy of a perturbation is derived according to the principles of mathematical entropy analysis and using a general definition of entropy amendable to physical phenomena such as thermal nonequilibrium and caloric and thermal imperfection. This normalization is shown to be closely related to the contemporary Chu energy normalization, expanding the range of validity of that normalization and clarifying the details of its interpretation. This relationship provides a basis for deriving other normalizations. Entropy analysis has also been applied to develop an entropy transport equation with which the entropy generation in a flow can be calculated.

The entropy norm is applied to predict the growth of instabilities in compressible boundary layers and was found to predict amplification consistent with the Chu norm. The norms were found to diverge in their predictions above Mach 5. The entropy norm was found to be more responsive to temperature gradients in the flow, which is a key factor in amplifying second-mode instabilities. This represents an advantage of the entropy norm over the Chu norm.

The norm has also been applied in POD analysis of two test cases. The first of these cases is a jet in supersonic crossflow, a well-characterized canonical case which is useful in evaluating the behavior of the entropy norm in cases with large temperature gradients. The entropy norm places more importance on these

temperature fluctuations than the Chu norm. The entropy norm has the advantage in reduced-order modeling in that such models will converge to an entropy-respecting solution.

Entropy production in highly compressible turbulence as it varies with critical flow parameters has been analyzed. Thermal conduction and nonequilibrium losses are found to be critical mechanisms of entropy production. Entropy is also demonstrated to behave monotonically even when turbulent kinetic energy does not describe the turbulent cascade. These findings provide a potential avenue for the development of robust turbulence models and analysis tools.

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Nomenclature

α	Spanwise wave number
α	Streamwise wave number
δ_{ij}	Kroniker delta
$\dot{n}$	Molar production/depletion rate via electron impact ionization
$\dot{w}$	Mass production/depletion rate
ϵ_i	Quantum energy level
η	Thermal conduction coefficient
$\hat{D}$	Characteristic vibrational energy
$\hat{I}$	First ionization energy
$\hat{z}$	Denotes a molar quantity
μ	Molecular viscosity
$\bar{z}$	Denotes a density-weighted time-averaged quantity
$\bar{z}$	Denotes a time-averaged quantity
ϕ, ψ	Entropy potential functions
ρ	density

σ	Molecular symmetry factor
$\mathbf{f}$	Conservative form flux function
$\mathbf{f}$	Entropy flux function
$\mathbf{q}$	Vector of conservative variables
$\mathbf{v}$	Vector of primitive variables
θ_r	Species characteristic rotational constant
θ_v	Species characteristic vibrational constant
$\theta_{e,n}$	Species and quantum level-specific constant
C_p	Specific heat at constant pressure
C_v	Specific heat at constant volume
D	Diffusion coefficient
E	Extrinsic energy
e	Specific internal energy
E_k	Perturbation kinetic energy
G	Gain in reference quantity
g_n	Species and quantum level-specific constant
H	Extrinsic enthalpy
h	Specific internal enthalpy or Planks constant
P or p	Static pressure
Q	Molecular partition function

q	Canonical partition function
R	Specific gas constant
S	Extrinsic entropy
s	Specific entropy
T	Equilibrium temperature
u, v, w	Cartesian velocities
x, y, z	Cartesian velocities
y	Mole fraction
z'	Denotes a density-weighted perturbation quantity
z'	Denotes a perturbation quantity
z^*	Refers to vibrational quantities calculated with translational-rotational temperature
z^{**}	Refers to vibrational quantities calculated with electronic temperature
z_e	Refers to the electronic energy mode
z_{int}	Refers to the rotational, vibrational, and electronic energy modes combined
z_r	Refers to the rotational energy mode
z_{tr}	Refers to the translational energy mode
z_v	Refers to the vibrational energy mode
z_{heavy}	Refers all species excluding free electrons

z_{ion}	Refers to ionized species only
z_{mol}	Refers to molecular species only
$z_{n,k}$	n refers to a given species and k refers a given thermodynamic mode

Chapter 1

Background

High-speed flight has been a goal for the aerospace industry for as long as it has existed. In the World Wars, the advantage provided by higher speeds drove innovations in structure, aerodynamics, and propulsion which raised the ceiling for aircraft velocity [1]. During the cold war, unmatched speed protected the SR-71, one of the most iconic high-speed systems ever built, from timely detection and ground-based defenses [2]. High-speed has been employed with some success in the commercial aviation industry as well. Notably, the BAC Concorde explored the possibility of commercial supersonic transportation until it was retired in 2003 [3]. Currently, several startups and entrepreneurial ventures [4, 5] are seeking to construct systems which build on the strengths of the Concorde, and NASA's low-boom efforts [6] are aiming to remove the technological limitations which restricted the Concorde's operational range. The fastest powered, in-atmosphere flight system constructed to date was the North American X-15, which was designed in the 1950's and saw its peak operation in the 1960's [7]. Though re-entry systems have achieved higher velocities, no human-operated powered flight system has flown faster than the X-15A-2's record of Mach 6.7 at 4,520 mph in 1968. In the years since, high-speed flight experienced a lull, at least in system production and implementation. When the X-15 retired no comparable system replaced it, and though re-entry and space-access systems often

achieve very high velocity during their return to earth, no human-operated system has achieved performance comparable to the X-15 without descending from orbit. This relative dearth in results has not been for a lack of trying. Since the X-15, at least 11 different programs have sought to build some form of reusable re-entry system, air-breathing high-Mach system, or hybrid launch system. Of these, only the X-37 has seen long-term use and many of the programs were cancelled before prototypes could be flown. This lull in technology deployment has also impacted space access. Half a century has passed since Apollo astronauts first landed on the moon, but entry systems today still rely on the same basic capsule configuration used in that program.

Despite these challenges, interest in high-speed flight has increased in recent years owing to investments from multiple sectors of the aerospace industry [8]. Research and development of space exploration technologies, commercial transportation, and national security have converged to an interest in the hypersonic flow regime. Space access and re-entry systems must traverse this flow regime as they move from stationary before takeoff to orbital velocity. High-speed systems can realize significant reductions in necessary ground infrastructure for time-sensitive earth-to-earth applications.

There are also important national security applications, as shown in Fig. 1.1, first published in The Economist [9] in 2019. In March of the same year, German foreign minister Heiko Maas cited high-speed systems as a key driver of world policy decisions [10]. In his testimony to the United States Senate Subcommittee on Emerging Threats and Capabilities, Under Secretary of Defense for Research and Engineering Michael Griffin emphasized this aspect of high-speed development, highlighting the emerging capabilities of other nations and the urgent need of the United States to reclaim its position as a technology leader in air-breathing high-speed systems [11].

Air-breathing space-access systems have been a technology goal for decades [12]. A concept presented by Palmer [13] and shown in Fig. 1.2 serves as a representative example of such systems. While re-usable rocket technology has significantly reduced launch costs in recent years [14], air breathing systems still promise utility beyond

that which can be provided by rockets. As Bradford et al.[15] point out in their 2004 paper proposing a two-stage system, not all space access missions are well-suited for a rocket-powered launch system. Rockets take off at times scheduled far in advance, and require large payloads to be economical. As an illustrative example, a mid-sized company that needs to send up a maintenance crew or equipment of fix an unexpectedly malfunctioning satellite would be well served by contracting a small launch system that carried only their cargo, delivered it to the exact location it needed to go, and could take off from any major airport. This in contrast to a heavy-lift rocket which would take off at a pre-scheduled time and would not necessarily deliver that payload to the precise orbit desired. In their contemporaneous analysis of a notional design and testing cycle for a two-stage system, Sawai et al [16] also cite this idea as motivation for their work. In essence, two-stage and hybrid launch systems, which are enabled by improved understanding of highly-compressible flow, are not necessary for current space access needs, but they are valuable for enabling an orbital economy which includes participants smaller than national governments and their contractors.

1.1 Technical Background

The high-Mach number flow regime is characterized by specific flow phenomena which makes designing for these conditions uniquely difficult. Each of the specific phenomena outlined here is the subject of numerous studies all on its own, and the following discussion is intended to serve as a high-level introduction to the technical problems associated with designing and validating high-speed flight systems. These topic areas will be given more detailed treatment as they become specifically relevant to this work, and associated references provide more detailed discussions into each of these problem areas.

As outlined by Anderson [17], these flows are characterized by thin shock layers, the presence of an entropy layer, high gas temperatures, increased coupling of viscous and inviscid phenomena, and eventually thermodynamic and chemical nonequilibrium

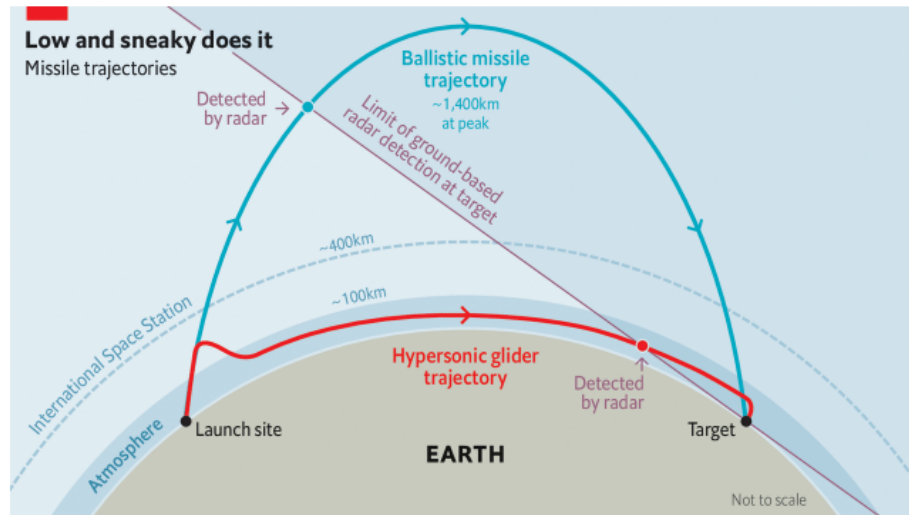


Figure 1.1: Illustration of hypersonic national security utility. Published April 6, 2019 in The Economist [9].

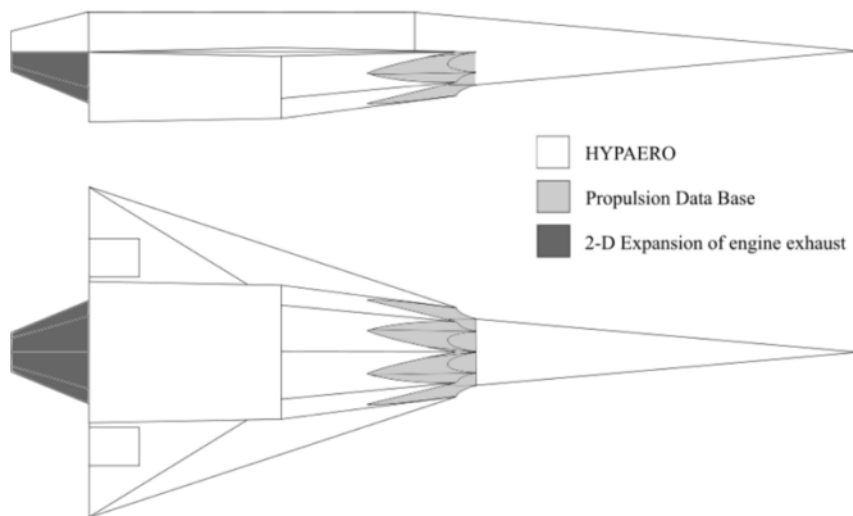


Figure 1.2: SPARTAN scramjet-powered space access system proposed by Palmer [13].

[17]. As Mach number increases, oblique shocks incline closer to the body. Because viscous heating expands gas in the boundary layer, the shock layer and the boundary layer tend towards overlap, which can complicate flows significantly. In regions where shock waves lie close to the body and where the flow through the shock is not deflected away from impinging on the body (such as near a stagnation point), high-entropy flow will be present near the body but outside of the boundary layer. This region is called the entropy layer. The entropy layer is inherently rotational per Crocco’s theorem [17], and its existence prevents self-similar boundary layer calculations from being applicable for many high-Mach number flows because the outer boundary condition can no longer be assumed to be uniform isentropic flow [18]. As exemplified in Ref. [19], the entropy layer can be fully engulfed by the boundary layer as the boundary layer develops, which introduces an additional instability mechanism when studying boundary layer stability for hypersonic flows. Moreover, enforcement of the no-slip condition requires flow to be nonisentropically slowed to stop. Slowing from a high Mach number to a stop recovers a significant portion of its total temperature. For reference, air flow at Mach 10 has a reference total temperature 21 times higher than the free stream, so recovering only half of it at an altitude of 80,000 ft would heat the boundary layer region to 2,200 K, which is well beyond the melting point of aircraft-grade aluminum alloys [20]. Prediction of laminar-turbulent transition in compressible flows is also uniquely challenging, and the typical stability and input-output analyses used by the aerodynamics community must be adapted for this regime [21].

Flow in this regime is also characterized by unsteady shock wave-boundary layer interactions and shock-shock interactions [22, 23], which significantly impact the heat and pressure loads on the body. On complex geometries, shockwave-boundary layer interactions (SWBLIs) can also generate flow features which advect downstream, creating even more complex interactions. A shock wave imposes significant adverse pressure gradient on the boundary layer, which can instigate flow separation and lead to secondary flow features such as vortices [24]. SWBLIs are often characterized by unsteadiness, which further increases their impact on any sort of final design, as the

elevated loads associated with the SWBLI are not guaranteed to be applied in the same place or at the same frequency over the whole flight regime, and interactions can yield lower-frequency oscillations which can approach critical structural frequencies. This type of interaction was found in numerical investigations of Mars entry descent and landing vehicles [25].

At very high Mach number, typical thermodynamic closures of the Navier-Stokes equations are no longer sufficient to characterize the chemical state of the flow. The calorically perfect assumption breaks down when thermodynamic energies become high enough that gas molecules become vibrationally and electronically excited. The excitation of these additional energy storage modes introduces nonlinearity to the relationship between temperature and internal energy. Moreover, thermodynamically-induced chemical reactions seed the flow with multiple chemical and ionic species, which change the gas parameters and require separate enforcement of conservation of mass for each species [26]. The differential form of the governing fluid equations with a three-temperature approximation is derived by Gnoffo et al. [27].

1.1.1 State of the Field

Despite these challenges, current timelines for fabrication of high-speed systems are ambitious. In a report prepared for the nonpartisan Congressional Research Service, a shared staffing institution whose role is to compile reports for legislators to inform policy, technology and global security analyst Kelley Sayler provides a comprehensive list of publicly-disclosed hypersonics development programs [8]. This report outlines a planned 2020 budget of 1.6 billion dollars in development of hypersonic systems targeting flight tests in the early 2020's. In a report for for the UN Office for Disarmament Affairs, Borrie et al. outline the hypersonics programs of the multiple nations, including the United States [28]. This account details an environment in which policy decisions are being made to drive development of systems forward quickly based on our current understanding of high-speed flow.

By contrast, academic study of high-Mach number flows has, for some time, focused heavily on very simple configurations designed to isolate individual flow phenomena. These are often called canonical configurations. Canonical configurations, many of which are described in detail by Gaitonde in Ref. [29], are purposeful abstractions of flow scenarios are used by researchers to separate the fundamentals of a flow response to a class of geometry from the specifics of an individual flight vehicle. By design, canonical flows are characterized by a small handful of geometric and flow parameters, and together constitute a rich library of data to which new methods and experimental techniques can be compared. Studying canonical cases provides an opportunity to apply very high-fidelity methods to a problems with a known solution, which is useful in identifying the underlying physics or in testing new methods and analysis paradigms. For example, Currao et al. identified Görtler instabilities in a transitional reflected shock wave on a flat plate using global diagnostics of an experiment and direct numerical simulation (DNS) [30]. The canonical configuration allowed the researchers to conclude that the reflected shock was inducing these instabilities, because there were no other geometric complexities to consider. Similarly, canonical configurations can be used to diagnose the energy content of specific shock-wave/boundary-layer interactions (SWBLIs) or boundary layer instabilities. Such an analysis was performed by Goparju et al. in ref. [18], where a flat plate with a blunted nose was used to study boundary layer stability, and Deshpande and Poggie [31], who used DNS to study the low-frequency instability of a compression ramp with sidewalls. In all of these cases, the simplicity of the canonical configuration allows the researcher to identify and study a specific physical phenomena in which they are interested.

While canonical configurations are extremely useful in developing analysis techniques and new knowledge of fundamental aerodynamic physics, there are drawbacks to this approach. Firstly, canonical configurations are often defined by a small number of geometric parameters. This can lead to canonical configurations omitting complicating factors in definition, but that are necessarily present in real systems

(even those those are notionally canonical). For instance, it is well-known that leading edge radius is an important parameter when considering boundary layer stability [32] and aeroheating [33]; however, most canonical computational studies omit this feature so as to not pollute the physics in which they are interested, despite every real system requiring a blunted leading edge for survivability. Moreover, these limitations also make experimental study of canonical configurations difficult. For example, very few studies consider compression corners to have a finite turning radius, but it was shown by Egorov et al. that the growth of second-mode instabilities in the boundary layer downstream of the compression corner is sensitive to the size of the re-circulation region in the corner, which in turn is a function of the corner radius [34].

1.1.2 Ground Testing Challenges

The difficulty of designing high-speed systems is further exasperated by the limitations on high-speed wind-tunnel testing. Achieving high Mach numbers in a wind tunnel has historically been a challenge. There are numerous types of high-speed testing facilities, and each achieves a different balance of test time, Reynolds number, Mach number, stagnation enthalpy, test-section size, and free-stream turbulence [35]. Arc-jet facilities achieve extremely high temperatures in a gas by arc heating it and then expanding the flow through a nozzle [36]. These facilities are used for testing thermal protection systems (TPS) for reentry because they can achieve the high enthalpy associated with reentry for long enough that the degradation of the TPS can be observed. They are also capable of using feed gases other than air, so they are good for simulating re-entry to other bodies in the solar system [37]. Shock tunnels generate high Mach number flows by rupturing a diaphragm which separates a high-pressure and low-pressure region of the working gas. These configurations come in different varieties each of which has benefits and drawbacks. Blowdown tunnels offer relatively high unit Reynolds numbers with relatively low operating costs [38]; however, they tend to have high free-stream noise and very short test times, requiring

instrumentation which can gather data in this short time and making them poor choices for studying low-frequency phenomena [39]. A related concept is the Ludweig tube, which uses a vacuum chamber, but does not include a high-pressure chamber. Recently, so-called quiet versions of this sort of configuration have been added as an experimental tool. These facilities seek to control the acoustic disturbances radiating from the boundary layer of the nozzle [40], which significantly reduces the pressure fluctuations in the test section [41] allowing for laminar flow over larger portions of the model. These facilities tend to be limited in test section size and therefore produce sub-flight Reynolds numbers based on the characteristic length of the model. Shock tubes are capable of generating extremely high enthalpies but have such short run times that they are not suited for aerodynamic research. They are however, useful for studying nonequilibrium gas dynamics which take place at such small scales [17]. There are also numerous permutations and specialized tunnel types, including those for studying highly compressible flows in a near vacuum or studying electric propulsion systems[42].

1.1.3 Numerical and Computational Methods

One important note to be taken from this discussion of high-speed ground testing capabilities is that no system can reproduce flight-relevant conditions long enough to capture low-frequency phenomena. Because of this, ground testing can not, on its own, fully validate the design of a high-speed vehicle. Instead, experimental and computational methods must be used. In such an effort experimental and computational methods produce results for a sufficiently similar case which is used to evaluate the efficacy of the computational method for the problem, and then the vetted computational methods are used to evaluate the realistic system. For realistic geometries, iterations on the initial design often use an inviscid code or a code with de-coupled viscid-inviscid capabilities. Euler (inviscid) solvers like CART3D [43] and panel codes like CBAERO [44] are used for compressible cases to quickly generate

force coefficients and other relevant performance data. For validation or analysis of potential problem areas, higher-fidelity methods which include the effects of viscosity are required.

Reynolds-averaged Navier-Stokes (RANS) solutions are the work horse tool for most of the aerodynamics industry [45]. These tools solve for the time-averaged flow field by assuming that turbulence is statistically stationary and then include an additional closure, called a turbulence model, that accounts for the changes to the mean flow caused by turbulence [46]. RANS has been used countless times for problems in all phases of the concept, design, and evaluation process. However, because they model turbulence instead of resolving it, and because they are inherently time-averaged, RANS calculations are insufficient to build an understanding of a problem for which the fundamental physics are not well-characterized. For these cases, RANS calculations must be evaluated against experimental results or higher fidelity computational methods as was done in Ref [47]. The highest-fidelity class of simulation available is direct numerical simulation (DNS) in which the analysis seeks to resolve all scales of the flow. Many authors additionally require DNS to use high-order, low-dissipation numerical methods [48] or exhibit specific favorable wave number modification characteristics [49]. DNS has been employed in high-speed aerodynamics for various applications. A few examples of DNS or DNS-assisted studies are found in Refs [50], [51], and [52]. DNS must resolve the smallest turbulent scales in the flow, the Kolmogorov scales [46], and this fidelity requirement translates directly to computational costs, making DNS cost-prohibitive for most applications. The middle ground between these two methods is Large-Eddy Simulations (LES) and the specific flavor of LES that will be considered in this work is implicit LES (ILES). ILES resolves large turbulent eddies but allows numerical dissipation from the spatial discretization of the Navier-Stokes equation to act as an effective turbulence model for eddies that would be smaller than the grid size. Because ILES ties the turbulent dissipation rate in the flow to the spatial discretization, it has been shown that the solutions of ILES computations are dependent on the choice of discretization scheme

[53]. ILES not only saves computational time in spatial resolution over DNS, but it also saves computational resources because the small grid spacing required by DNS force the solver to take smaller time steps for stability, especially for explicit time-marching schemes. In this way, ILES allows the user to achieve a high level of fidelity with a coarser discretization in space and time [54] than is possible with DNS. ILES has been demonstrated to be a favorable method for tackling problems for which the restrictions of RANS preclude a meaningful answer, but for which DNS would be too computationally expensive. It is also a good candidate for examining laminar-turbulent transition because it resolves the large-scale turbulent eddies which form at the onset of transition [55].

Taken as a whole, the study of highly-compressible flows is a difficult and multifaceted problem. It is also one of the most critical areas required for the advancement of high-speed flight. Aerodynamic loading defines the boundary conditions for structural and control system design problems, and the variety of salient physics which may be encountered in this regime combined with the complexity of fluids problems in general strongly suggests the pursuit of high-speed flight stands to benefit from broadly applicable, physics-based analysis tools. In this work, a novel entropy-based method for characterizing unsteady fluctuations is derived and characterized. The normalization is applied to stability analysis and proper orthogonal decomposition (POD), a representative modal decomposition technique, to demonstrate how this normalization can help to unify the analysis of high-speed flows and elucidate the physics in question. The mathematical arguments made in deriving the norm are then extended to derive a relationship for calculating and budgeting the entropy production in compressible nonequilibrium flows. This relationship is demonstrated by examining the entropy generation in isotropic nonequilibrium turbulence.

Chapter 2

Literature Review

2.1 Matrix Normalizations

It is common in fluid analysis to decompose a flow into mean and perturbations quantities. This technique is used to study the dynamics of flow systems both for the purposes of analysis of an unsteady flow solution, such as the case with decomposition methods, and to predict potential instabilities from a base flow. It is also common that these methods require taking an inner product of flow quantities with one another, often taking perturbations from different temporal manifestations or spatial positions and systematically operating on each of them. Mathematically, this process is an L^2 norm, but for compressible fluid dynamics problems a Euclidean norm does not necessarily represent the total magnitude of a perturbation. This problem is drawn into focus by examining a simple vector norm, such as the one used to calculate energy at a point given the primitive flow quantities. A Euclidian norm is uncontroversial for flows where a single quantity is of interest, but for flows where multiple flow quantities are to be considered simultaneously it is necessary for a definition of the L^2 norm to exist which is both physically meaningful and dimensionally consistent. For incompressible flows, kinetic energy is a straightforward and appropriate measure of perturbation magnitude because the decoupling of thermodynamics from kinematics

allows for a robust statement of its behavior. In application, it is an unweighted norm of the velocities,

$$E_k = \frac{\rho}{2} \int u^2 + v^2 + w^2 dV \quad (2.1)$$

For compressible flows, thermodynamic phenomena interact with kinematics and so a measure that considers only kinematics is no longer appropriate. In this regime the unweighted L^2 norm of the full set of flow variables is not dimensionally consistent or physically meaningful. It is therefore necessary for some kind of relevant pre-multiplication of the perturbations of variables be employed before the Euclidean magnitude can be evaluated. This problem extends beyond a vector norm at a point to the inner product between perturbations in general, and the generalized form of the premultiplying factor is a matrix normalization. Matrix normalizations are weighting schemes in the form of symmetric, positive-definite matrices that define an inner product of flow variables. An appropriately-chosen matrix norm unifies the scaling and dimensionality of a problem. Often, these normalizations are constructed so that the resulting inner product is representative of some real-world quantity. The most common normalization scheme in use for compressible flows today is the Chu energy norm [56],

$$E = \frac{1}{2} \int \left(\frac{R\bar{T}\rho'^2}{\bar{\rho}} + \bar{\rho} u'_i u'_i + \frac{\bar{\rho}C_v T'^2}{\bar{T}} \right) dV \quad (2.2)$$

where the overbar denotes a time-averaged quantity and the prime denotes a fluctuating quantity. This may be written in matrix notation as,

$$\bar{E}_{vv} = diag \left(\frac{R\bar{T}}{\bar{\rho}}, \bar{\rho}, \bar{\rho}, \bar{\rho}, \frac{\bar{\rho}C_v}{\bar{T}} \right) \quad (2.3)$$

$$E = \frac{1}{2} \int \mathbf{v}'^T \bar{E}_{vv} \mathbf{v}' d\tau \quad (2.4)$$

where $\mathbf{v} = [\rho, u, v, w, T]^T$. Chu derived this approach in 1965 as a quantity representative of and dimensionally consistent with energy in order to provide a basis for examining the stability of perturbations in compressible flows. When using the primitive flow variables, the Chu norm is a diagonal matrix, meaning the covariance between different variables of different perturbations are zero. In the incompressible limit it converges back to a normalization of kinetic energy. The Chu norm has been used successfully to analyze compressible flows with modal decomposition and for stability applications. Hanifi et al. [57] provide an example of a case where this matrix norm is applied for linear stability analysis, as well a thorough discussion of its derivation. The Chu norm is currently the most widely-accepted standard method for modal decompositions of compressible flows [58] and has seen wide applicability in the literature. Shrestha et al. [59] use it to evaluate transition of hypersonic boundary layers behind a trip through DMD modes. Ryu et al. [60] used the Chu norm in their analysis seeking to identify instability waves in high-speed jets. It was also used by Sun et al. to normalize compressible cavity flows in a resolvent analysis [61].

Despite its record of successful use, the Chu norm includes assumptions and simplifications which are not clearly motivated from the physical scenarios it is now employed to study. As described in its derivation, the Chu norm justifies the omission of the pressure work done by the perturbation through assumptions that are valid for analysis of boundary layers, but not in general. For this and similar reasons, the scheme is generally referred to, even in its original presentation, as a functional definition of energy, which aims to describe the mean intensity of fluctuation in a disturbance. Energy is also not necessarily the only quantity against which the flow can or should be contracted. Colonius et al. [62] showcase this in particular, using an energy, enthalpy, and pressure norm as well as multiple weighting schemes and

comparing the convergence of reduced-order models derived from those POD modes. In principle, there are no limitations on what can and cannot be used as a basis for normalization in POD, so long as the matrix chosen is symmetric and positive-definite. In the literature it is often observed that normalizations are chosen to be diagonal matrices. This is often computationally expedient but is not a mathematical requirement. It is often preferable that the matrix norm be based on a quantity that is of interest to the physical scenario being studied. The precise reasons for this preference are dependent on the application of the matrix norm, but in general the requirements of modal analysis and predictive methods coincide due to their similar mathematical constructions. Here, entropy is examined as a basis for matrix normalizations for compressible flows based on its role in driving unsteady processes and its ubiquity.

2.2 Entropy

As dictated by the second law of thermodynamics, the entropy of a closed system must never decrease. Entropy may be understood as a measure of the quality of the energy in a system- its ability to do useful work. Increasing global entropy corresponds to an overall decrease in the quality of energy, and when a system achieves its maximum entropy state it can no longer do any work. Entropy is important in many fields and may be expressed in many different ways. Fields such as economics even employ quantities analogous to physical entropy, which seek to describe behaviors of societally-constructed systems akin to those seen in nature. Of interest here are the independent but related concepts of entropy in a thermodynamical system and in mathematics. Entropy is often considered to be a measure of the disorder of a system, but this definition is not necessarily useful for engineering applications. This is because disorder often has no tangible definition, and no clear connection to the quantities that are actually of use in physical systems. Moreover, it is observed in nature that matter often spontaneously assumes forms which appear to be highly

ordered, such as crystal structures or biological cells, in seeming contradiction to the principle of increasing disorder. For practical applications, a more appropriate description of entropy would be that entropy is a measure of how uniformly energy in a closed system is distributed, and the second law of thermodynamics states that energy can spontaneously disperse, but cannot spontaneously concentrate. The popularization of the disorder interpretation is speculated in the literature to be a result of Boltzmann's infatuation with Darwin's theory of evolution [63]. This fascination with Darwin's theories combined with his exploration of an ideal gas system led Boltzmann to consider dispersal of energy to be synonymous with disorder [64]. The interpretation based around disorder does not require invocation of other physical laws, and easier to form analogy with, hence its popularity. The understanding that entropy most fundamentally describes the distribution of energy in a system is critical both for the motivation and execution of the described work.

As suggested by its definition, entropy is a universal property of all systems and matter. Problems such as ablation, propulsion, and flow ionization require that any tools used to analyze them be amendable to a wide range of physical principles. Entropy has well-established applications in virtually every field of physics and chemistry. Energy sciences [65] and even cosmology [66] have foundational principles based on entropy. Entropy can also be defined statistically for cases where this definition is appropriate. The continuum definition of entropy is emergent from the statistical definition applied over a sufficiently large sample [67]. Importantly, entropy definitions applied in various fields, including the thermodynamic entropy applied here, are expressions of entropy that include the terms relevant to the application. Each of these are comparable to one another, and the definitions from one field can be generalized to include contributions from another should the application require it. Therefore, entropy can be defined in wakes or very thin shock layers as well as perfect gasses in a continuum. Features that are usually significant challenges for flow calculations, such as finite-rate chemistry also contribute to entropy generation in a well-characterized manner. For example, Garbet et al. [68] have demonstrated

a method for calculating the entropy production rate of turbulence in magnetized plasmas in the kinetic regime and in the fluid regime. Owing to this generality, a valid and complete definition of entropy can be derived for any valid flow scenario. Entropy is also closely related to one of the most common applications for matrix normalizations, stability.

2.2.1 Entropy and System Stability

Stability in aerodynamic contexts is often assumed to refer to the propensity of a viscous laminar boundary layer to transition to turbulence. While this is an aspect of flow stability, it is not the whole of it. An adequate discussion of the strengths and shortcomings of stability evaluation methods requires a more complete context for stability in fluid flows, so a brief discussion of the discipline is in order. Sengupta [69] describes instability in terms of the gap between governing equations and the physical manifestation of systems. In essence, they describe solutions to conservation laws that satisfy existence and uniqueness, but which are never observed in nature. The solutions that cannot be manifested physically are described as unstable. The definition of Sengupta is presented in the historical context of the experiments of Reynolds [70], which identified such a scenario. This definition is intuitive, but requires some clarification. For instance, this definition would seem to include expansion shocks in the Euler equations, since that phenomena can be described mathematically but is never observed physically. Discrepancies between the predictions of conservation laws can result either from solution instability, but also from incompleteness of the governing equations. A self-similar laminar boundary layer at high Reynolds number is unstable because the equations used to model it do not consider surface roughness, free-stream disturbances, or any of the other small imperfections that would nudge the laminar boundary layer infinitesimally and irrevocably away from its self similar shape. In the case of the expansion shock, the Euler equations are incomplete in that they do not consider viscosity, whose presence

precludes such occurrences. The expansion shock could also be found nonphysical by invoking the second law. The invocation of entropy provides a significant level of insight into the circumstances that lead to instability, the evaluation of stability of a system, and the dynamic behavior of systems moving about a steady-state. This relationship is drawn in to close focus when considering extrema principles, which are locally valid special cases of the second law that provide insight into system dynamics beyond that provided by conservation laws. In fact, the importance of entropy for system stability is widely recognized outside of the context of laminar-turbulent transition. This is especially true in the study of high speed flows, where entropic arguments have been used to examine the stability of shockwave structures [71], particularly in supersonic inlets where the stability of the shock structure is critical for operation [72]. This paradigm is also closely related to the typical method of energy tabulation, as is also shown by Xu et al. [73], who derived a minimum energy dissipation principle for flows as a special case of the minimum entropy principle of Prirogine [74]. In fact, generalized nonequilibrium thermodynamics provides a set governing principles by which localized stability problems of all kinds may be analyzed using entropy [65]. In this context, it may be suspected that the aerodynamics community's preference for understanding stability as a phenomena of energy is valid as a special case where energy is proportional to entropy and therefore serves as its surrogate. In essence, conservation laws such as the first law of thermodynamics define the space of possible configurations a system may assume, and entropy defines the most probable (and therefore the macroscopically manifested) path through that space. Because stability concerns itself with predicting the path of the evolution of a flow, it follows that entropy is an important aspect of the problem.

Extrema principles of entropy generation are often used to analyze dynamic systems. These are the minimum [74] and maximum [75] entropy generation principles. They are theorems derived from evaluating the first and second law of thermodynamics in specific circumstances, and describe nonequilibrium systems such as fluid flows. The minimum entropy generation principle, valid for non-equilibrium

dissipative systems near steady-state, states that any spontaneous change in the configuration of the system must decrease the local entropy generation rate of the system. Therefore, the system is only stable if the entropy generation rate is at a minimum relative to nearby possible configurations. Essentially, small perturbations in a dissipative system at a point of minimum entropy will die out in time as the gradient of entropy generation drives the system back to its original configuration. Because the shockwaves at a supersonic engine inlet, for example, constitute a dissipative system, this principle is very useful in evaluating their stability. The maximum entropy generation principle states that open systems evolve in such a way as to maximize the global entropy generation [76]. This is seemingly in direct opposition to the minimum entropy generation principle, but these two are in fact not at odds, as their domain of application does not overlap [77]. Borrowing terminology from nonequilibrium thermodynamics, the minimum entropy generation principle states that a system will adjust its thermodynamic forces to the configuration of minimum entropy generation required to satisfy its steady thermodynamic fluxes, while the maximum entropy generation principle states that, given thermodynamic forces, a system's fluxes will evolve to the configuration of maximum global entropy generation. As examples, an inlet shock structure will achieve the minimum entropy generation required to satisfy its downstream boundary condition [72], but a flow subject to a gravitational force, cooling at the upper boundary, and heating at the lower boundary whose fluxes are not prescribed will evolve to generate as much entropy as possible [78]. Still, because of the specificity required to invoke either principle directly, attempts to use these principles predicatively rather than diagnostically have been met with frustration [79]. These principles are also scale dependent and the minimum principle specifically is only valid locally, rather than globally [80]. Some systems may even undergo transient periods where they obey the one principle and then switch to another. A system far from equilibrium may evolve according to the maximum principle by adjusting its fluxes, but as it approaches equilibrium these fluxes may stop changing, and the internal thermodynamic forces

of the system will change so as to minimize entropy generation. Being theorems which govern the behavior of systems only within their respective regimes, entropy extrema principles are generally insufficient to recover constitutive relationships for a system. Within the field of energy sciences, these principles and their specific interpretations is a subject of significant debate [77]. Nevertheless, these theorems are sufficient to clearly establish a causal relationship between the stability of a system, its boundary conditions, and its entropy state.

Historical Development of Entropy Analysis

Entropy as a concept was developed alongside the rest of classical thermodynamics before the quantum-mechanical aspects of gas dynamics were understood. As such, there exist parallel definitions of the quantity for numerous fields which evolved out of the original schools of classical thermodynamics. These schools were foundations of their own fields, and so the study of entropy has evolved largely as it is useful to these fields. For instance, the treatment of entropy for fluid dynamics and CFD is descended from Rudolf Clausius and the Berlin school, while Maxwell's namesake demonic paradox is the foundation of entropy in the context of computational science. The work of Gibbs has informed biology and chemistry, while Boltzmann's statistical approach has informed particle physics and plasma dynamics. Each of these field's descriptions is an expression of the second law of thermodynamics, and painstaking work of many researches has consistently demonstrated this fact. Nevertheless, the historic stratification in the greater scientific community's understanding of entropy is often a source of confusion. The work presented here relies on the equivalence between entropy as defined in classical thermodynamics and as described by modern thermodynamics informed by chemistry and quantum mechanics. The connections and overlaps between these two approaches to entropy will be highlighted as they appear.

2.3 Compressible Turbulence Analysis

Canuto describes classical turbulence analysis as the prediction of Reynolds stresses [81]. This often necessitates the prediction of decaying turbulent kinetic energy (TKE) [46], which is the kinetic energy contained in turbulent eddies. Conventional wisdom holds that turbulent kinetic energy monotonically decays in turbulence. The influence of compressibility in the temperature field is contextualized by invocation of the Huang Strong Reynolds Analogy, developed by Huang to replace the classical Strong Reynolds Analogy [82]. This analogy postulates that temperature fluctuations in compressible turbulent flows are a function of velocity fluctuations in a compressible flow. This assumes a perfect anticorrelation to the coupling between velocity and temperature in compressible turbulence.

Despite the limitations of methods centered on energy, the approach centered on Reynolds stresses, the Reynolds analogy, and turbulent kinetic energy has seen widespread success owing to the robustness of its assumptions for conditions which had been examined in the literature [83], [48]. The apparent robustness of this approach has staved off alternate approaches for most of the history of the aerospace industry. In recent years, renewed interest in high-speed flows combined with improved experimental and computational capabilities have begun to identify the shortcomings of such approaches for high-speed flows. Ziefu’s analysis found the Reynolds analogy acceptable for first-order approximations of wall-bounded flows but unacceptable for general applications, and their findings ”strongly suggest moving toward more advanced turbulent heat transfer models consistent with thermodynamic laws” [84]. Eyink and Drivas identified theoretical inconsistencies in their purely mathematical analysis applying Onsager’s approach to compressible turbulence, which is interpreted by Hellinger et al. as evidence that a conservative kinetic energy cascade may not generally exist for compressible flows [85]. Simultaneously, the community is re-evaluating its approach to turbulence modeling, as second-moment closures may now be computationally tractable [45].

2.4 Modal Decomposition of Compressible Flows

Matrix normalizations are often also employed in the context of modal decomposition. Modal decomposition methods decompose a data set defined across two dimensions into a series of weighted basis functions, similar in principle to a Fourier series expansion of a function. Modal decompositions are a useful tool in isolating salient physics because the partitioning of flow features into separate modes can help to isolate the individual features which combine non-linearly and manifest as the flow solution. Modal decompositions are also often a basis for reduced-order modeling, as the weighted modes they produce can be partially reconstructed to approximately represent the original field. These properties have made modal decompositions a popular tool for compressible flows. Their ability to reduce data to dominant modes can be useful both in isolating the salient physics from complex interactions, thus helping to bridge the gap between canonical cases and application, and in reducing the important aspects of large data sets to a tractable size. Though most often applied to data coherent in space and time, modal decompositions can be used for data sets defined along other parameters. Tang et al. used modal decomposition to examine the mean response of the flow around an X-34 as it moved through its flight envelope using a response-surface model derived using dominant response modes [86]. For these reasons, these methods have become very common within the aerodynamics community. There are multiple modal decompositions commonly used in the field of aerodynamics. Dynamic mode decomposition (DMD) [87], Proper Orthogonal Decomposition (POD) [88] and spectral proper orthogonal decomposition (SPOD) [89] are all commonly used in applications, and are described thoroughly in the associated references. POD is the method focused on here, though matrix norms are similarly applicable to many decompositions.

Recent work with modal decompositions in high-speed flow has focused most on attempting to increase the fidelity of design tools by incorporating reduced-order models derived from these decompositions into them. Decker et. al [90] demonstrate

such a technique for both analytically defined cases and CFD results. In this study, POD was one of just three methods used in a wider procedure aimed at training models to predict flow features at lower computational cost than simulating them. A similar framework is presented by Ghoman et al. [91], who used POD as a critical component in an optimization process for high-speed vehicle designs. Reduced-order models are not only capable of predicting behavior of systems throughout an operational envelope, they are also an attractive potential option for predicting unsteady behavior without expensive simulations, since many unsteady behaviors are too low-frequency to capture well in experiment. Chen et al [92] use an algorithm with training data derived from CFD to predict flutter characteristics of a diamond airfoil using a reduced-order-model constructed from POD modes.

Modal decompositions are just as often employed to interrogate complex physics as they are to construct reduced-order models. These techniques are also not limited to computational data. Cottier et al. [93], [94] demonstrate this by employing SPOD to study the unsteady characteristics of an unsteady cylinder-induced SWBLI captured through Schlieren imaging. Tumuklu et al. study a flow in thermochemical nonequilibrium using POD, and found that the impact of nonequilibrium on the shock-shock interaction structure induced by a double cone was reflected in dominant POD modes [95]. This study applied POD to results generated through direct simulation Monte-Carlo, which is a technique commonly used for rarefied fluid flows. This study did not employ a matrix normalization. Modal decompositions are usable for any data set expressed or expressible as a matrix. As such, they are not limited to aerodynamics problems. Klock and Cesnik apply POD to the thermal properties of hypersonic vehicle structures to develop reduced order models to predict vehicle performance [96]. While this requires data derived from aerodynamics to serve as a boundary conditions, the modal decomposition itself is applied to structural data.

2.4.1 POD Algorithm

The description of POD here follows that of Taira et al. [88]. POD is usually applied to mean-subtracted data, though the algorithm can be applied to any data set. The goal is to generate a set of weighted orthonormal modes which, when recombined, will recover the original data set. This is expressed mathematically as

$$q(\xi, t) - \bar{q}(\xi) = \sum_j a_j \phi_j(\xi, t) \quad (2.5)$$

where $\phi_j(\xi, t)$ are the modes and a_j are the weighting coefficients. The weighting coefficients are taken to be dependent only on time and the modes only dependent on space. This splits the problem into two lower-dimensionality problems which may be treated separately. From this point forward, the perturbations will be denoted as x , as in

$$x(\xi, t) = q(\xi, t) - \bar{q}(\xi) \in \mathbb{R}^N, \quad t = t_1, t_2, \dots, t_M \quad (2.6)$$

POD specifically seeks to find the fewest possible modes required to reconstruct the original set of perturbations. This means that POD seeks to unevenly-distribute modal dynamic content such that the dominant modes contain as much of this content as possible. When considered as a series expansion this corresponds to an expansion which converges quickly. This is solved as an eigenvalue problem where λ_j are the eigenvalues of R , the covariance matrix of x . This can also be understood as an optimization problem where the mean of the projection of R onto itself is minimized.

POD is constructed so that the fewest possible number of modes can be used to adequately describe the original data set. This manifests as an uneven distribution of dynamic content, favoring a few dominant modes in which the relevant dynamic content is concentrated. Another interpretation of this property is that POD returns the fastest-converging expansion of the original flow data. The decomposition may be

found through an eigenvalue problem where λ_j are the eigenvalues of R , the covariance matrix of x , as in

$$R\phi_j = \lambda_j\phi_j, \quad \phi_j \in \mathbb{R}^N, \quad \lambda \geq \dots \geq \lambda_N \geq 0 \quad (2.7)$$

$$R = \sum_{i=1}^M x(t_i)x^T(t_i) = \frac{XX^T}{M} \in \mathbb{R}^{N \times N} \quad (2.8)$$

This formulation is an optimization problem where the mean of the projection of R onto itself is minimized.

POD can also be performed via the snapshot method. The snapshot method is employed in situations where the number of rows of X is significantly greater than the number of columns. This is the case for CFD data, where a mesh may contain millions or billions of points, but the time domain of interest only usually contains a few hundred to thousand of data cross-sections. The snapshot method can greatly reduce the size of the eigenvalue problem for these cases compared to the above approach.

There is an alternate approach which may be taken to perform POD on data sets where the number of rows of X is significantly greater than the number of columns. This is usually the case for CFD data because the size of a typical mesh, often hundreds of millions to billions of data points, is much greater than the number of temporal manifestations, which typically number in the hundreds to thousands for a large data set. The snapshot method can significantly reduce the size of the eigenvalue problem compared to the above approach, and is formulated according to

$$X^T X \psi_j = \lambda_j \psi_j, \quad \psi_j \in \mathbb{R}^M, \quad M \ll N \quad (2.9)$$

$X^T X$ is of size $M \times M$ and shares its nonzero values with XX^T . From this, the POD modes can then be calculated using the results of the eigenvalue problem,

$$\begin{aligned}\phi_j &= X\psi_j \frac{1}{\lambda_j} \in \mathbb{R}^N, \quad j = 1, 2, \dots, M, \quad \Phi = [\phi_1 \quad \phi_2 \quad \dots \quad \phi_M] \in \mathbb{R}^{N \times M}, \\ \Psi &= [\psi_1 \quad \psi_2 \quad \dots \quad \psi_M] \in \mathbb{R}^{M \times M}\end{aligned}\tag{2.10}$$

An alternative approach to the snapshot POD is to calculate the modes via a singular value decomposition (SVD). This approach is seldom taken, due to the computational cost of directly taking the SVD. Nevertheless, the SVD and eigenvalue decomposition of diagonalizable matrices are closely related, where the SVD is performed according to

$$X = \Phi \Sigma \Psi^T \tag{2.11}$$

$$\Phi = X \Psi \Lambda^{-1/2} \tag{2.12}$$

where Σ in the SVD contains the singular values of σ_j of X . These are also the squares of the eigenvalues of $X^T X$. Φ and Ψ are identically the eigenvectors of XX^T and $X^T X$ respectively. For cases where the SVD can be found, the POD modes can be calculated directly

From an algorithmic standpoint, POD is agnostic to the physics of the problems it is employed to analyze, and so the definition of modal dynamic content must be clarified. In POD, the "modal dynamic content" takes the units and dimensionality of the covariance matrix $X^T X$. The eigenvalues then correspond to the portion of the contracted dynamic content described by its corresponding mode. It is here that the application of matrix normalizations for POD becomes critical. Without normalization, POD of compressible flows is the decomposition an L^2 norm of dimensionally inconsistent quantities. This norm is not meaningful, and because the physical meaning of the eigenvalues (and therefore the modes) is inherited from $X^T X$, it is not clear what is described by the modes of such an analysis. This

is compounded when considering POD for the purpose of reduced-order modeling. The reduced-order model is intended to recover the relevant dynamics of the flow by combining the dominant few modes, but if the dynamics are not adequately described by the eigenvalues then there is no way to guarantee the algorithm will return modes describing the dominant physics of the problem. An appropriately weighted contraction ensures that the covariance matrix, and therefore the modes, can be interpreted through the physics of the problem. For instance, if the entropy norm presented here is used then the eigenvalues would describe the portion of the entropy of the unsteady flow contributed by a given mode.

2.5 Boundary Layer Instability Growth

One of the earliest applications of matrix norms was for the analysis of compressible boundary layers. The recovery of the high free-stream enthalpy of hypersonic flows in the viscous boundary layer is responsible for the large heat fluxes experienced by hypersonic vehicles. For this reason, characterizing the behavior of compressible boundary layers is a topic of interest to the high-speed community. Anderson [17] describes the compressible boundary layer equations for an ideal, calorically perfect gas, while Dorrance [97] describes a dissociating boundary layer with potential chemical interactions with the wall, and Bitter and Shepherd [98] describe a laminar boundary layer in thermochemical non-equilibrium. Given the role of laminar-turbulent transition in amplifying the thermal loads experienced by a system in flight, stability analysis and transition prediction have been a focus of study for some time. Stability-type analysis is one of the most computationally tractable and popular tools for examining this problem.

Methods which operate on this framework take a time-invariant flow as their input and seek to evaluate whether and how unsteady phenomena might emerge were that base flow observed. These techniques are often employed to evaluate whether or not a flow would be expected to undergo laminar-turbulent transition [99], but they can

also be used to study specific flow behaviors such as the instability of shear layers [100].

2.6 The Jet in Crossflow

The jet-in-crossflow is a canonical case often studied for aerodynamic and propulsion applications. The sustained interest in the jet-in-crossflow is exemplified by Margaston [101], a retrospective analysis of fifty years of prior research, itself published nearly three decades ago. The jet-in-supersonic-crossflow is a permutation of this case which introduces shock-expansion structures and an SWBLI to the already-complex canonical flowfield [102]. Heister and Karagozian provide estimates for key flow properties which may be solved algebraically [103]. The jet in crossflow has garnered even more interest from the community since CFD has become commonplace, and is often used to compare methods to each other [47], [104].

The supersonic jet-in-crossflow is characterized by the complex interactions between the shock structure caused by the jet and the jet itself. The incoming jet flow obstructs the free-stream flow creating a bow shock which instigates boundary layer separation and creates a re-circulation region at the wall just upstream of the jet. This feature advects around around the jet near the wall creating a horseshoe vortex. Inside the jet region there is barrel shock and a mach disk, which act to regulate the pressure of the under-expanded flow. These features are shown schematically in Fig. 2.1 and are described in more detail in [105].

Chemical reactions and heterogenous flow (where the jet and free-stream have different compositions) are often studied in the context of the jet in crossflow. The temperature increase of the shockwave caused by the jet can be sufficient to instigate chemical reactions such as combustion in the jet flow [106]. The Jet in crossflow can represent a practical challenge for CFD, as the dynamic regions of the flow are spread out across the domain. Steady CFD with turbulence modeling can and has been used to examine the configuration [107], but because turbulent mixing, combustion,

and other dynamic behaviors are hallmarks of the jet-in-supersonic-crossflow, it is often more informative to use time-accurate methods [108]. Examples of the jet-in-supersonic crossflow may be further categorized based on whether the boundary layer upstream of the jet is laminar, as in [109], or turbulent, as in [110]. The interference of the jet can also trip the flow from laminar flow to turbulence, as was observed in Ref. [111], further complicating the interaction. The dynamics of the upper plume region are generally independent of the state of the flow at the wall, but the SWBLI at the base of the jet outlet demonstrates different behavior depending on the state of the incoming boundary layer.

The jet-in-supersonic-crossflow was chosen as a case study to demonstrate POD with the entropy normalization due to the ease with which significant temperature gradients could be introduced to the flow. The free-stream, flat-plate wall, and jet inflow each have a thermodynamic reference or boundary condition. This test case is also a compact showcase of dynamic behaviors which can be resolved with relatively affordable simulations compared to many unsteady compressible phenomena. Finally, the jet-in-crossflow facilitates the study of multispecies flow, as in the case where the properties of the two inflows are different. Because the entropy normalization is specifically intended to facilitate analysis of multispecies flow, a case with a long history for studying inhomogeneous is a reasonable starting point to characterize its behavior.

2.7 Isotropic Turbulence and Taylor-Green Flow

Compressible turbulence is a critical area in high-speed flow research. Turbulence and transition drastically increase the surface heating experienced at high speed, and turbulent mixing is critical to the operation of air-breathing high-speed propulsion systems. Analysis of full scale systems usually relies on turbulence models to capture the effects of turbulence, but these models must be constructed and calibrated using more detailed simulations or experimental observations. Characterization of

turbulence in flows is often performed in terms of the turbulent kinetic energy [46]. Turbulent kinetic energy is, as the name would suggest, a purely kinematic quantity. In order to handle thermal considerations, some version of the Strong Reynolds Analogy is usually employed, which provides an estimated relationship between the turbulent thermal fluctuations and the kinematic behavior of the flow [82]. This approach is useful in some applications, but is fundamentally limited by one-sided dependence. These methods assume that the kinematics of the flow so overwhelmingly dominate the thermodynamics that this simplification is acceptable. Entropy analysis provides a rigorous method of evaluating this assumption by exhaustively bookkeeping all of the losses in the flow. This provides a mechanism to evaluate the relative importance of each loss mechanism, and by tandem analysis of the turbulent flow field itself, information can be gleaned about the validity of such kinematics-first approaches to compressible turbulence.

Another avenue which must be examined is the impact of thermal and caloric imperfection and thermochemical nonequilibrium on compressible turbulence. These phenomena have been examined in some detail in the literature. Neville et al. [112] studied the potential for vibrational nonequilibrium to damp temperature fluctuations in turbulent flows and found that such damping is possible. Bitter investigated the importance of vibrational nonequilibrium to boundary layer stability, and found that it could have stabilizing or destabilizing effects depending on the Reynolds number, gas characteristics, and disturbance frequencies [98]. Ramanathan et al. [113] found that, even for high temperatures and in considering caloric imperfection, viscous dissipation still dominates the production of turbulent kinetic energy. Even so, there are gaps in the existing knowledge base which entropy analysis is well-positioned to fill. Namely, the quantification of losses by nonequilibrium mechanisms must be calculated, and their impact on the losses associated with other modes must be compared to their values.

Analysis of isotropic turbulence is one of the most fundamental canonical analyses of compressible turbulence. Isotropic turbulence analysis considers a cube whose

sides are each 2π in length, resolved by a uniform computational domain with periodic boundary conditions applied to each face. The case of canonical isotropic turbulence is a widely utilized problem to build fundamental understanding of turbulent phenomena. One major advantage of the case is that, by construction, there is no base flow which needs to be considered. This means that, rather than using Reynolds or Favre averaging to decompose the equations into a mean and perturbations, the equations can be taken in their whole, unmodified form and all of the dynamics may be attributed to turbulent fluctuation. Isotropic turbulence and related analyses are the simplest possible turbulence problems, and so are a natural starting point for new turbulence analysis paradigms.

For simulation of isotropic turbulence, the velocity field is initialized as a set of overlapping Fourier modes of different wave numbers, with the special case of a single mode referred to as a Taylor-Green vortex. The Taylor-Green vortex is the very simplest possible turbulence analysis. The exact definition of a Taylor-Green vortex for compressible flows is debated in the literature, and many references specify an initial velocity and temperature field as an additional requirement for the Taylor-Green vortex in compressible conditions. Despite this, literature also confirms that the initial thermodynamic (density and temperature) perturbation field has very little impact on the resultant turbulent decay, suggesting the initial field should be chosen so as to make the simulation computationally tractable [114]. The analysis of a single-mode (Taylor-Green) perturbation or more complex isotropic turbulence is a natural starting point for analysis aimed at fundamental understanding of compressible turbulence. The lack of a mean flow simplifies the execution of the simulation and removes sometimes-restrictive post-processing steps.

Compressible isotropic turbulence and Taylor-Green flow has been examined extensively in the literature. Peng and Yang examined the impact of compressibility on vortex fields, and their work is notable for demonstrating the relatively small influence on initial thermodynamic conditions (conditions of pressure, temperature, and density) given the Taylor-Green initial velocity conditions [115]. They also

demonstrate the lack of monotonicity of TKE as turbulence decays at higher Mach numbers. This study examined Mach numbers between 0.5 and 2. Lusher used the compressible Taylor-Green vortex as a test bed for low-dissipation shock capturing techniques [116]. The Taylor-Green vortex is often a test bed for computational capabilities and new methods, as exemplified by its inclusion in the International Workshop on Higher-Order CFD Methods [117]. Munafo et al. use a Taylor-Green vortex and isotropic turbulence to demonstrate high-order methods for multicomponent and nonequilibrium gases [118]. It is well-known that the compressible Taylor-Green vortex violates the monotonicity of turbulent kinetic energy, which is taken as given at lower speeds. The fundamental nature of the problem lends itself well to examination of the effects of high-temperature and thermal non-equilibrium effects, as were analyzed by Ramanathan [113] and Neville [112] respectively. Gallis et al. also applied DSMC to the simulation of isotropic turbulence and found structures in DSMC simulations at high Mach number not present in comparable DNS [119].

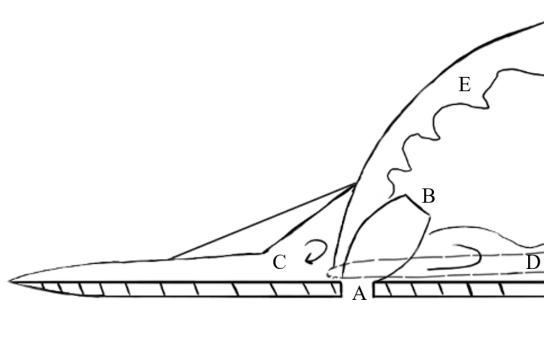


Figure 2.1: Schematic of a jet in supersonic crossflow. Features of interest are the jet opening (A), the Mach disc (B), the SWBLI recirculation region (C), the horseshoe vortex (D), and the jet-bow shock interface (E)

Chapter 3

Matrix Normalization about Entropy

Data Source Statement

The derivation of the ideal gas entropy normalization and discussion of its relationship to the Chu norm was originally written for a submission to *Theoretical and Computational Fluid Dynamics* which is currently under review for publication, and has been adapted for inclusion here.

3.1 Molar Entropy of a Gas

In typical aerodynamic situations entropy is usually thought of in terms of its classical, continuum definition. Unfortunately, the description of entropy provided by classical thermodynamics is not necessarily sufficient for all applications. In order to develop a more robust framework, a general approach for fluid dynamics problems will be identified and common simplifications can be derived as they become relevant. This problem can be approached from a statistical mechanics standpoint, as in Ref. [120], but generally this type of approach can't bridge the gap between a representative system and the physics of interest. Rather, this gap can be bridged by employing

the molecular partition function for a gas. The canonical partition function, denoted here as q , is a necessary precursor to the molecular partition function and describes the number of energy states available to a gas molecule [121], and is related to the energy levels of states according to

$$q = \sum_i e^{-\beta \epsilon_i} \quad (3.1)$$

where $\beta = \frac{1}{kT}$ and ϵ_i is an individual energy level. The molecular partition function, Q , can be derived from the canonical partition function according to,

$$Q = \frac{q^N}{N!} \quad (3.2)$$

for indistinguishable molecules. The molecular partition function provides a framework by which all of the modes of energy storage available to individual molecules in a gas can be treated independently. This will ultimately allow for permutations of the entropy norm to be derived by simplifying the generalized model. For gas molecules there are four such modes, translation, vibration, rotation, and electronic excitement. The molecular partition function can be decomposed as,

$$Q = Q_{tr} Q_r Q_v Q_e = Q_{tr} Q_{int} \quad (3.3)$$

where Q_{int} is the product of the vibrational, rotational, and electronic partition functions. As suggested by eqn 3.3, the translational partition is treated somewhat differently from the other components. The reason for this will become clear through the discussion of entropy as derived from the partition function. As described by Gökçen [26], the molar entropy and energy can be described in terms of the partition function according to

$$\hat{s} = \hat{R} \left[\ln \frac{Q}{N} + 1 + T \frac{\partial(\ln Q)}{\partial T} \right] \quad (3.4)$$

$$\hat{e} = \hat{R} T^2 \frac{\partial(\ln Q)}{\partial T} \quad (3.5)$$

Combining the decomposed partition functions with the definition of entropy allows the entropy to be decomposed as follows,

$$\hat{s} = \hat{s}_{tr} + \hat{s}_r + \hat{s}_v + \hat{s}_e \quad (3.6)$$

The specific partition functions are

$$\begin{aligned} Q_{tr} &= V \left(\frac{2\pi m k T}{h^2} \right)^{\frac{3}{2}} \\ Q_r &= \frac{1}{\sigma} \frac{T}{\theta_r} \\ Q_v &= \frac{1}{1 - e^{-\frac{\theta_v}{T}}} \\ Q_e &= \sum_{n=0}^{\infty} g_n e^{-\frac{\theta_{en}}{T}} \end{aligned} \quad (3.7)$$

where θ_r , g_n , and θ_{en} are species-specific constants and σ is the symmetry factor, which is 1 for homonuclear molecules and 2 for heteronuclear molecules. It should also be noted that for monotomic species Q_r and Q_v are unity, since single atoms have no degrees of freedom in those modes. It can be observed from the definitions of the partition functions that all of the modes depend only on temperature except for the translational mode. This translational mode is responsible for the pressure dependence of the familiar ideal gas entropy equation. Because the translational entropy contribution is ubiquitous, it can be split into a thermal and nonthermal component, which allows for consistent treatment of the entropy normalization. The entropy norm's dependence on the thermodynamic closure (an example of which is the ideal gas law) is limited to this translational term. The electronic partition function also requires additional clarification. Each term in the infinite sum of the electronic partition function corresponds to an excited energy level an electron may achieve. For an isolated atom in a vacuum there are an infinite number of excited states that an electron can take, whose energy levels asymptotically approach the element's ionization potential above which the electron escapes the atom, yielding a free electron

and an ion [122]. In real applications, the presence of external species reduces the effective ionization potential of the atom, truncating the series. For most engineering applications, this series is truncated at a number of microstates chosen *a priori*, after which increasing modes do not significantly alter the value of the thermodynamic quantities. In plasma dynamics, where the electronic properties of the substance are a central focus of study, more sophisticated methods must be employed to evaluate the excitation of the electrons of each species. Fig. 3.1 shows a sample of the trends in electronic excitation as temperature increases. Here, the most prevalent excited species correspond to the first few terms of the sum in Eq. 3.7.

There is one more important relationship which can be demonstrated from the definitions of $\hat{e}$ and $\hat{s}$. By differentiating each with respect to temperature, it can be shown that

$$\frac{\frac{\partial e}{\partial T}}{\frac{\partial s}{\partial T}} = T \quad (3.8)$$

regardless of the form or value of the individual partition function. This is a generalization of the classical relationship $\delta s = \frac{de}{T}$ for systems with heat transfer but no work. This relation is also important in simplifying the generalized entropy norm.

3.1.1 Behavior of Partition Components

It can quickly be observed that the four-partition description of energy or entropy is much more involved than the descriptions commonly used in practice. Indeed, this description is usually too difficult to work with and too computationally costly to use in practice, and applied analysis relies on a description of the thermodynamic variables which has been simplified to some degree from this expression. The appropriateness and limitations of such simplifications can only be evaluated by examining the unsimplified case to examine which terms may be dropped or approximated and

under which circumstances. The entropy of N_2 as a function of temperature is shown in Fig. 3.2.

It is clear from this example that at modest temperatures the vibrational and electronic components of entropy (as well as energy) are very small compared to the rotational and translational components. For these cases, it is often convenient to omit these terms entirely. Another reason that omitting these terms is an attractive simplification can be found by examining the molar energy associated with each mode for the case of an ideal gas,

$$\begin{aligned}\hat{e}_{tr} &= \frac{3}{2}RT \\ \hat{e}_r &= RT \\ \hat{e}_v &= \frac{\hat{R}\theta_v}{e^{\frac{\theta_v}{T}} - 1} \\ \hat{e}_e &= \frac{\hat{R}}{Q_e} \sum_{n=1}^{\infty} g_n \theta_{en} e^{-\frac{\theta_{en}}{T}}\end{aligned}\tag{3.9}$$

The energy of the translational and rotational modes is more mathematically convenient than the other two modes. For modest conditions, the vibrational and electronic terms can be dropped, significantly simplifying the problem with nearly no impact on the quality of the solution. The omission of these terms combined with the choice of the ideal gas equation of state recovers the familiar relations for energy and entropy from classical thermodynamics. These relations allow for the introduction of constant specific heats, C_v and C_p , as well as γ to better account for the properties of solutions of ideal gases, such as air. These specific values could be determined by taking a proportionate sum of the specific gas constants of the constituents of the solution, but the constant gas composition renders this exercises an unnecessary

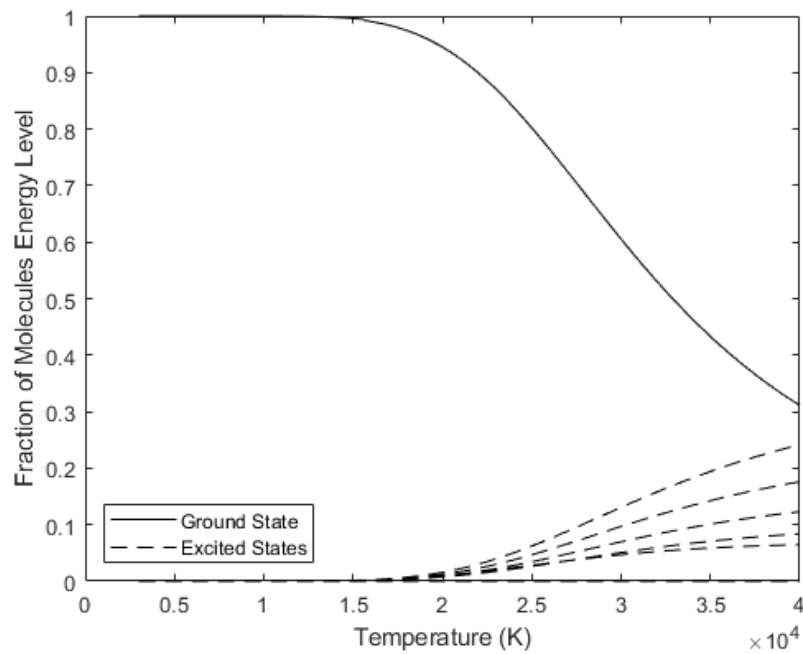


Figure 3.1: Sample of the excitation state distribution calculated for hydrogen showing the decreasing relevance of additional electronic states

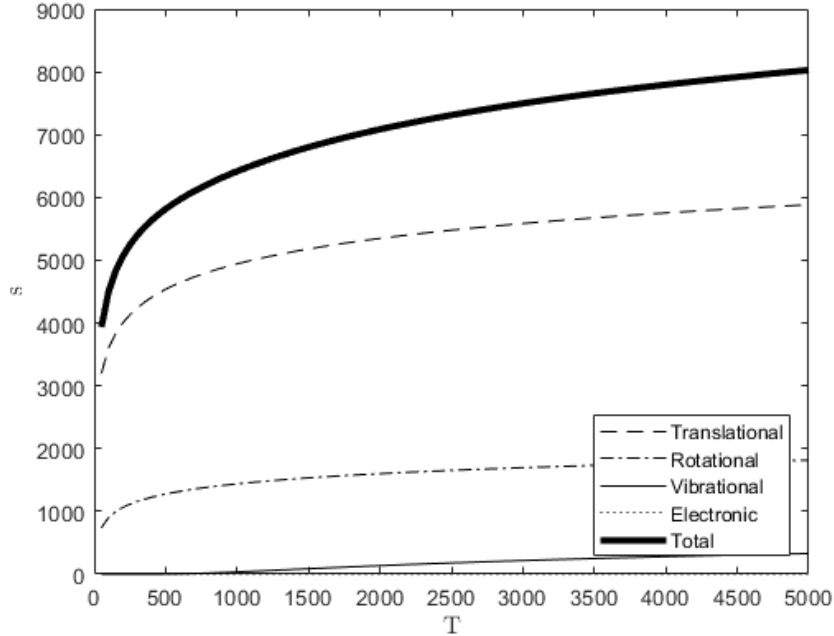


Figure 3.2: Entropy of each energy storage mechanism in diatomic Nitrogen at standard atmospheric pressure. Entropy is dominated by the rotational and translational components in this regime.

complication. For completeness, it should be recognized that this expression of the rotational and translational energy contributions assumes these modes are saturated, which is nearly universally true for engineering applications, but must be evaluated as an assumption for very extreme cases, such as the simulation of instabilities in comet tails as in Ref. [123].

As temperatures increase, the vibrational and electronic modes cease to be negligible; however, the explicit treatment of these additional modes using the relationships for energy and entropy from the partition functions is still more complicated than the other modes. Moreover, the increasing prevalence of these modes precedes the introduction of chemical reactions to the flow field for most gases. For these reasons, it is often expedient to maintain the framework established for the calorically perfect case. For these cases, the specific heats are functions of temperature, but the other relationships remain the same. Often, this analysis paradigm will still omit electronic excitation because it remains small up to the tens of thousands of degrees Kelvin for most stable diatomic gases. Caloric imperfection does not necessitate thermal imperfection, so these gases still obey the ideal gas law. In this regime, the vibrational energy storage mode is excited, but is still in equilibrium with the other modes, so there is no need to employ a vibrational temperature. For nonequilibrium flows, most engineering tools either rely on a three-temperature expression of the governing equations or a two-temperature statement of the governing equations. Three-temperature expressions generally consider the translational and rotational modes to be in equilibrium with one another and the other modes are tracked independently. Two-temperature models, which offer a computational cost savings, consider one of the following cases: the translation and rotation modes are in equilibrium and vibration and electronic modes are in equilibrium, or the vibration and rotation are in equilibrium, the translation is independent, and the electronic is omitted.

As temperature increases further, chemical reactions may begin to occur within the gas. At this point it becomes necessary to treat the gas as a mixture of individual

constituents because the composition, and therefore the properties of the gas, can change through unsteady processes. Chemical reactions within a flow must be treated with a separate model. Commonly used nonequilibrium chemistry models are those of Park and Gupta [124]. The onset of chemical nonequilibrium significantly increases the cost of simulations because of the introduction of the coupled chemical model and the necessity of re-calculating the gas properties at each step.

For flows at high temperature but very low pressure, the time scales of the energy transfer between thermodynamic modes approach the time scales of the kinematic of the flow. This means that these internal modes can no longer all be assumed to be in equilibrium with one another. When this occurs, the flow is considered to be in thermal nonequilibrium. In thermal nonequilibrium, an additional governing equation must be added to the PDE conservation law system for each mode that is not in equilibrium with the others, and an additional temperature is needed to close the system. In thermal nonequilibrium flows, some modes may still be considered to be in equilibrium with one another. It is generally accepted that the translational and rotational modes are saturated for all but very low temperatures, so these modes are usually taken to be in equilibrium with one another when considering diatomic gases. The vibrational and electronic modes may be considered to be in equilibrium with one another, or they may be considered to be independent. For certain gases, the translational, rotational, and vibrational modes may each be treated independently while the electronic contribution is still so low as to be negligible. Flows in thermodynamic and chemical nonequilibrium are generally associated with re-entry, and represent the ceiling of complexity for engineering flows considered here. Alternative thermodynamic closure relationships such as the Van-der-Waals equation may be employed instead of the ideal gas law for any of the regimes described here.

3.2 Mathematical Entropy

Having discussed entropy in the physical sense as an ever-increasing property of the universe driving energy away from itself so as to render it useless in extracting mechanical work, entropy will now be defined in the purely mathematical sense. In systems of ordinary (ODE) or partial (PDE) differential equations, it is common for multiple solutions to exist which satisfy a steady-state solution of the system. When using mathematical models to make predictions, especially approximate methods like those common in engineering applications, the possibility of multiple solutions poses a problem. The possibility of multiple solutions emerging from computational tools is problematic because it is usually unclear if all of these solutions can be physically manifested. This problem arises because these systems of equations are constructed using only conservation laws, which on their own are an insufficient description of any physical system. The second law of thermodynamics is required to evaluate the physicality of the solution. Unfortunately the second law does not fit cleanly into most computations, leaving two choices. Solutions could be evaluated using physical entropy after the fact, which would be impractical, expensive, and would not address the issue of convergence to erroneous solutions. Alternately, problems can be constructed using methods which converge to the entropy solution of the system, found using the mathematical entropy of the equations. The mathematical entropy, expressed as an entropy-flux pair for conservation laws, are properties of the equations only. For PDE systems which model real phenomena, the physical and mathematical entropies have been found to coincide for many systems. Whether this link is coincidental or a manifestation of physical laws has never been proven [125], but the agreement is sufficiently common that it is generally assumed in engineering contexts to be the latter. In either case, the coincidence of mathematical and physical entropy for a system is extremely advantageous, as solving for the mathematical entropy solution guarantees a solution consistent with the physical entropy of the system being modeled. Identifying these entropy-flux pairs from scratch is challenging. No reliable

method exists for identifying these pairs for systems of conservation laws like those employed in aerodynamics calculations. Nevertheless, the evaluation of agreement between the physical and mathematical entropy does not necessarily require the exact form of the mathematical entropy to be known a priori, so long as physical entropy is defined. One can simply conduct the mathematical analysis using the formulation for physical entropy, and if the resultant modified system does not exhibit the properties of an entropy solution, disagreement can be inferred.

The role of mathematical entropy can be demonstrated using a canonical system of conservation laws according to the formulation outlined by Tadmor [126], beginning with the statement of a general conservation law.

$$\mathbf{q}_t + \text{div}(\mathbf{f}(\mathbf{q})) = 0 \quad (3.10)$$

For purposes of analogy to the Navier Stokes equations studied here, the flux term in equation 3.10 may be split into a viscous and inviscid flux, which may be done without loss of generality. Written in generalized index notation, this becomes

$$\mathbf{q}_t + \mathbf{f}(\mathbf{q})_x^{(I)} - \mathbf{f}(\mathbf{q})_x^{(V)} = 0 \quad (3.11)$$

Here, the t represents time and x represents the considered spatial dimensions. For now, the values of the solution and flux terms are left symbolic, but they will be discussed in greater detail later. For demonstration purposes, the flux term will be left together, and the equation will remain in a form similar to the Euler equations.

A quantity $S(q)$ is defined to be an entropy function of the system. The criteria for a valid entropy function are outlined by Parsini et al. [127]. This entropy function must be convex, as in

$$S_{qq}A = [S_{qq}A]^T \quad (3.12)$$

for

$$A(\mathbf{q}) = \mathbf{f}_{\mathbf{q}}(\mathbf{q}) \quad (3.13)$$

We seek to transform these equations into an equivalent symmetric form. To accomplish this, the introduction of the entropy variables is required. These variables are defined as the vector derivative of the entropy function with respect to the conservative variables of the system, where the original conservation law is defined as

$$\frac{\partial}{\partial t} \mathbf{q} + \frac{\partial}{\partial x} \mathbf{f}(\mathbf{q}) = 0 \quad (3.14)$$

The mapping between the conservative and primitive variables must be one-to-one for the analysis to continue, which itself requires the convexity of the entropy function. This allows the conservative variables to be taken as functions of the entropy variables, denoted $\mathbf{w}$ and specifically defined in the upcoming sections, as in $\mathbf{q} = \mathbf{q}(\mathbf{w})$. If this condition is met, the governing equation can be expressed in its symmetric form,

$$\frac{\partial}{\partial t} \mathbf{q}(\mathbf{w}) + \frac{\partial}{\partial x} \mathbf{g}(\mathbf{w}) = 0 \quad (3.15)$$

where $g(w) = f(q(w))$. Symmetry in this context refers to the symmetry of the Jacobians of the fluxes are symmetric, as in

$$H(\mathbf{w}) = q_w(\mathbf{w}) = H^T(\mathbf{w}) \quad (3.16)$$

and

$$B(\mathbf{w}) = g_w(\mathbf{w}) = B^T(\mathbf{w}) \quad (3.17)$$

The convexity of the entropy function requires the existence of an entropy flux function, F , defined according to

$$S_{\mathbf{q}}^T \mathbf{f}_{\mathbf{q}} = F_{\mathbf{q}}^T \quad (3.18)$$

From this, entropy potential functions can be defined,

$$\mathbf{q}(\mathbf{w}) = \nabla_w \phi(\mathbf{w}), \quad \phi(\mathbf{w}) = \langle \mathbf{w}, \mathbf{q}(\mathbf{w}) \rangle - S(\mathbf{u}(\mathbf{w})) \quad (3.19)$$

$$\mathbf{g}(\mathbf{w}) = \nabla_w \psi(\mathbf{w}), \quad \psi(\mathbf{w}) = \langle \mathbf{w}, \mathbf{g}(\mathbf{w}) \rangle - F(\mathbf{u}(\mathbf{w})) \quad (3.20)$$

The potential functions are an important tool for the development of the entropy stable and entropy conservative methods commonly employed by modern CFD solvers, such as those described in Refs. [128], and [129]. For the present analysis, the calculation of the entropy variables and the convexity of the entropy function are of greater concern.

For cases where it is not known, the entropy function may be found through the method of vanishing viscosity. That is, we take the solution vector $\mathbf{q}$ to be $\mathbf{q} = \lim_{\epsilon \rightarrow 0} \mathbf{q}^\epsilon$, with the modified governing equation

$$\mathbf{q}_t^\epsilon + \text{div} \mathbf{f}(\mathbf{q}^\epsilon) = \epsilon (P \mathbf{u}_x^\epsilon)_x \quad (3.21)$$

where

$$P S_{qq}^{-1} = [P S_{qq}^{-1}]^T \quad (3.22)$$

Multiplying through by w and taking the limit of $\epsilon \rightarrow 0$ yields the entropy inequality,

$$\frac{\partial}{\partial t} S(\mathbf{q}) + \frac{\partial}{\partial x} F(\mathbf{q}) \leq 0 \quad (3.23)$$

Because Eq. 3.10 permits multiple weak solutions, the entropy inequality is necessary to identify those solutions which are of physical interest. For scalar conservation laws, any symmetric function may be an adequate entropy function S . For systems of equations this is not necessarily the case. The connection between physical and mathematical entropy, and thus the utility of the entropy solution, requires that the expected entropy function provided by thermodynamics is also a

convex entropy function of the PDE system. Owing to the framing of the problem, mathematical entropy is usually taken to be the negative of physical entropy. This discrepancy reflects the different goals of the analyses: mathematical entropy is used to limit the value of a solution to within a certain range and is usually expressed as decreasing in all time, while physical entropy must increase according to the second law. When the absolute values of the physical and mathematical entropy agree, these are equivalent expressions of the same phenomenon from two equally valid perspectives.

Summary

Entropy is observed to be a critical quantity for governing the dynamic behavior of systems, and has been employed in this capacity successfully in numerous fields, including aerodynamics. The universal applicability of the second law of thermodynamics makes entropy a natural choice for analysis of many different kinds of systems, especially those which may incorporate principles from historically separate areas of study. Mathematical entropy analysis is a key tool in ensuring the physicality of CFD solutions, and so it is only natural that entropy should continue to be of interest in analyses beyond generating a base flow, to modal decompositions, reduced-order modeling, and instability prediction.

3.3 Description of the Entropy Norm

In this section, a family of entropy normalizations is derived. These normalizations are permutations of the same analysis technique, whose details depend on the specific set of physics being considered (caloric perfection vs imperfection, thermal equilibrium or nonequilibrium, etc.). Analysis will begin with the case of a single-species, calorically and thermally perfect gas in equilibrium. This case is the direct analog of the Chu norm, so it can be used to examine the properties of the entropy analysis

and its relationship to Chu’s energy framework. After these relationships have been established, the generalized entropy norm will be presented. Because there are many ways the specifics of a problem may be handled by the user, the author does not attempt to specifically describe every permutation of the norm. Instead, a template norm will be provided into which the end user can drop the specific thermodynamic relationships they use in their analysis. This is aimed at allowing users to easily use the same closure relationships at all steps of their analysis. This also allows for equivalent relationships, such as the multiple curve fits often used for the vibrational and electron specific heats of gases, to be easily substituted for one another without needing to repeat derivations.

3.3.1 A Calorically Perfect Ideal Gas

The derivation of the calorically and thermally perfect entropy normalization utilizes the definition of entropy familiar in classical continuum thermodynamics. Like the Chu norm, all versions of the entropy norm require pressure temperature and density to be positive to guarantee that the matrix is positive-definite. In reality this restriction is immaterial, because these are also requirements of physicality for a flow. The calorically perfect norm is chosen as a starting point for this analysis because many of the components used in its derivation are already widely employed in other aspects of CFD. As will be discussed next, this derivation is also a blueprint for the more general normalizations which will be derived next, which include multiple species and are amendable to caloric and thermal imperfection, as well as thermal nonequilibrium.

The formulation of the ideal gas entropy normalization is performed according to the entropy analysis presented by Tadmor [126], which was also employed by Fisher and Carpenter [130]. The general approach of this derivation is to differentiate the quantity of interest with respect to mathematically convenient intermediate variable sets and use the chain rule to convert the Jacobian of entropy in terms of one variable

set to another. Perturbations in entropy can be linearized such that the covariance of perturbations in two separate manifestations of the flow (expressed as perturbation vectors in a variable set of choice) with the mean-referenced entropy norm as an intermediate multiplier will yield the entropy contained in the fluctuation required to get from one perturbation state to the other. To begin, the target variable set will be the conservative variables used by many CFD solvers, which represent the quantities which are directly governed by the conservation laws of fluid flows. The primitive variables, so named because they are the most elementary form of flow quantities, will be used as an intermediate. As an intermediate step in the derivation, the entropy variables, $\mathbf{w}$, will also be derived. These variables describe the state of the flow referenced to thermodynamic entropy. There are infinitely many variable sets which may be used in this or similar manipulations of the flow equations, but these three variable sets are easy to move between, easy to understand, and common in applications. Using the chain rule of calculus, one can map from one variable set to another by mapping the known quantities in one set to an intermediate set, and then analytically map the intermediate set to the desired set. The entropy variables can be derived as the rate of change of entropy with respect to the primitive variables multiplied by the mapping from the primitive variables, $\mathbf{v}$ to conservative variables, $\mathbf{q}$,

$$\frac{\partial S}{\partial v} = S_v = \left(R - s, 0, 0, 0, -\frac{\rho R}{(1 - \gamma)T} \right) \quad (3.24)$$

$$S_q = S_v \mathbf{v}_q = \frac{\partial S}{\partial \mathbf{v}} \frac{\partial \mathbf{v}}{\partial \mathbf{q}} = \mathbf{w}^T = \left[C_p - s - \frac{u^2 + v^2 + w^2}{2T}, \frac{u}{T}, \frac{v}{T}, \frac{w}{T}, -\frac{1}{T} \right] \quad (3.25)$$

This expression can be used with the Navier Stokes to develop a statement of the second law of thermodynamics. Integrating this expression over an arbitrary domain yields the Clausius-Duhem inequality,

$$\int_{\Omega} \mathbf{w}^T \left(\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial(\mathbf{f}_j - \mathbf{f}_j^{(v)})}{\partial x_j} \right) dV = \frac{dS}{dt} \leq 0 \quad (3.26)$$

This can also be interpreted as a statement of non-linear stability for the Navier-Stokes equations. The entropy variables are a complete set and the Navier-Stokes equations can be expressed completely in terms of the entropy variables. Due to the non-linearity of the mapping between the entropy and conservative variables, some operators such as averaging are not commutative between the two. A statement of the Navier-Stokes in terms of the entropy variables can be written in symbolic form as,

$$A_o \frac{\partial \mathbf{w}}{\partial t} + A_1 \frac{\partial \mathbf{w}}{\partial x} - \frac{\partial}{\partial x} \left(A_2 \frac{\partial \mathbf{w}}{\partial x} \right) = 0 \quad (3.27)$$

The coefficients of this statement of the Navier-Stokes equations map from the conservative to entropy variables. In particular, the symmetric positive-definite operator A_0 satisfies the specific requirements laid out for the entropy normalizations,

$$A_0^{-1} = \frac{\partial^2 S}{\partial q_m \partial q_n} = S_{qq} \quad (3.28)$$

Now that the term of interest has been identified and described its value can be ascertained. Once again the chain rule can be used to determine the form of the mapping using the primitive variables as intermediaries. First, the matrix

mapping of the entropy variables to the primitive variables can be determined by differentiating the former variable set with respect to the latter. Because the rate-relationships between the entropy variables and the primitive variables are known, and the relationship between the primitive and conservative variables are known, the previously unknown relationship between the entropy and conservative variables can be expressed as their product. This relationship is the entropy normalization S_{qq} ,

$$S_{qq} = \mathbf{w}_q = \mathbf{w}_v \mathbf{v}_q \quad (3.29)$$

Now that S_{qq} has been evaluated, the inner product described earlier can be evaluated. The values of the matrix Jacobians $\mathbf{w}_v$ and $\mathbf{v}_q$ are provided in Appendix A. The derivation of these quantities are also the beginning of the entropy analysis of the compressible Navier-Stokes. The mathematical entropy for the Navier Stokes is convex, and its Hessian, S_{qq} is symmetric and positive-definite [130],

$$\mathbf{w}^T \frac{d\mathbf{q}}{dt} = \mathbf{w}^T \frac{\partial \mathbf{q}}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial t} = \mathbf{w}^T S_{qq}^{-1} \frac{d\mathbf{w}}{dt} \quad (3.30)$$

The entropy norm can then be applied as an exact definition of entropy provided sufficiently small perturbations in the conservative variables. This takes the form,

$$S = \frac{1}{2} \int \mathbf{q}'^T \bar{S}_{qq} \mathbf{q}' d \quad (3.31)$$

3.3.2 Application for Modal Decompositions

For modal decomposition applications, S_{qq} can be calculated at each point in the domain based on the time-averaged flow quantities there. This is effectively a linearization of entropy perturbations expressed in the conservative variables,

$$\mathbf{w}' = \bar{S}_{qq}\mathbf{q}' + O(\mathbf{q}'^2) \quad (3.32)$$

The mean-valued $\bar{S}_{qq}$ matrix is then used in the same way the Chu normalization is employed in contemporary modal decompositions. For a continuum this would correspond to the differential entropy of the perturbations at a point in space, but for discrete data as exist in CFD solutions this corresponds to the perturbation entropy in the volume whose solution is represented by the grid point. Including $\bar{S}_{qq}$ in the covariance matrix calculation of POD modes where the independent variables are the conservative variables produces a POD algorithm whose singular values represent the fraction of the entropy of the total unsteady behavior described by the corresponding mode. By seeking to concentrate this quantity in the dominant few modes, this POD would seek to describe the dominant irreversible mechanisms in its dominant modes.

Entropy satisfies the requirements of a matrix norm for stability analysis and modal decomposition. The entropy normalization is ready to be implemented in this form, but before doing so it is worthwhile to evaluate its thermodynamic consistency with the Chu normalization as well.

This version of the entropy norm produces a 5×5 matrix at each grid point, which makes the storage and application 5 times more expensive than for the Chu norm. In exchange for this trade-off, this normalization operates in the primitive variables which are most common for CFD solvers. However, as will be shown the entropy norm can also be expressed in a form directly analogous to the Chu normalization. Before this, it is informative to explore the properties of the entropy norm as compared to

the Chu norm in cases where their reference quantities, entropy and energy, are both appropriate.

3.3.3 Theoretical Comparison with the Chu Norm

As discussed above, many modern applications of modal decomposition use a normalization based on the total energy contained in a perturbation. In considering a normalization based on a new thermodynamic quantity it is therefore important to consider the relationship of the new normalization those currently being employed in the industry. It has been demonstrated empirically that energy and enthalpy demonstrate increasingly undesirable behavior as a flow becomes dominated by the effects of compressibility [92]. Therefore, though the entropy normalization is developed with the intent of being applied to compressible flows, it is valuable to examine the behaviors of both of these quantities to establish expectations for their behavior in application.

Valid solutions to the full Navier-Stokes equations satisfy the Clasius-Duhem inequality and therefore the Second Law of Thermodynamics. This inequality is not enforced as a separate conservation law, but the presence of viscous dissipation guarantees this to be a direct consequence of the governing equations. Solutions that neglect viscous dissipation can be found mathematically, but those that decrease global thermodynamic entropy are considered nonphysical. A definition of thermodynamic entropy is presented where the equality condition indicates a reversible process,

$$Tds \geq de + \frac{P}{\rho^2}d\rho \quad (3.33)$$

3.3.4 Special Case: Incompressible Flow

For applications such as hydrodynamics or low-speed aerodynamics the incompressibility assumption is often invoked to reduce the complexity of the problem.

Incompressibility contends that density changes within the flow are so small as to be effectively zero, and so density may be treated as a local constant. The first consequence of the incompressibility assumption is the simplification of the continuity equation to a statement that the velocity field must be divergence-free. Incompressibility is often said to de-couple temperature from the rest of the Navier-Stokes equations. Mathematically, the removal of an unknown from the system reduces the number of equations required to close the system. This can be explained physically by virtue of the fact that changing density is the means by which the flow can exchange kinetic and thermodynamic energy, and therefore the need to track internal energy is removed when density is fixed. The second law of thermodynamics must still be enforced, so it is often still of interest to examine the energy state of the flow. This can be accomplished by contracting the momentum equations with the velocity to give,

$$\frac{\partial \rho \left(\frac{1}{2} u_i u_i \right)}{\partial t} + \frac{\partial \rho u_j \left(\frac{1}{2} u_i u_i + \frac{P}{\rho} \right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \frac{1}{2} u_i u_i}{\partial x_j} \right) - \mu \left(\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right) \quad (3.34)$$

Based on the definitions of e_0 and h_0 , this may be combined with energy conservation of the flow to produce an equation describing the transport of internal energy in the incompressible flow field,

$$\rho \frac{De}{Dt} = \mu \left(\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\frac{C_p \mu}{Pr} \frac{\partial T}{\partial x_j} \right) \quad (3.35)$$

which describes the increase in internal energy due to viscous dissipation of kinetic energy and the redistribution of internal energy due to heat transfer within the flow brought about by internal temperature gradients. Incompressibility also has implications for the definition of entropy since incompressible fluid elements do no work on their surroundings, nor can work be done on them,

$$ds \geq \frac{de}{T} = C_v \frac{dT}{T} \quad (3.36)$$

It is seen that the pressure dependency has been removed from the inequality, thus directly linking entropy, internal energy, and temperature. Because the internal energy and temperature are shown to be governed by the dissipation of kinetic energy, the dissipation of kinetic energy is a suitable surrogate for entropy in the special case of an incompressible flow. Taking the case where dT is small, such that T is effectively constant and the process is nearly reversible such that the relationship can be considered an equality, these three quantities are linearly related,

$$\delta s = \frac{\delta e}{\bar{T}} = C_v \frac{\delta T}{\bar{T}} \quad (3.37)$$

Consequently, in the case of a linearized analysis of incompressible unsteady flows such as that employed in modal decomposition, internal energy and entropy are interchangeable in their physical interpretation. In POD, the flow normalization considers individual flow realizations to be the sum of perturbations and a constant mean; the dynamics of the perturbations are analyzed by first contracting them in an L^2 norm against the base flow, which is taken to be constant. In tabulating perturbation energy, Chu's norm implicitly tracks perturbation entropy as well for the incompressible case and by extension, is an approximation of entropy for cases where compressibility effects are sufficiently weak.

This can also be shown by re-deriving the entropy normalization by contracting about the primitive variables rather than the conservative variables. Beginning with an expression of the entropy contraction mapping changes in the conservative variables to entropy. The form of the normalization is found by expanding this to a mean and small perturbations. Choosing the perturbations to be in terms of the primitive variables gives,

$$\frac{\partial S}{\partial t} = (\mathbf{w} + \frac{\partial \mathbf{w}}{\partial \mathbf{v}} \mathbf{v}')^T \frac{\partial}{\partial t} (\mathbf{q} + \frac{\partial \mathbf{q}}{\partial \mathbf{v}} \mathbf{v}') \quad (3.38)$$

Because only the perturbation terms are of interest, all quantities including a mean may be dropped. The remaining terms collapse via the chain rule to the hessian of entropy with respect to the primitive variables, which is the entropy matrix normalization. In this form, the entropy norm is denoted S_{vv} ,

$$\frac{\partial \mathbf{w}^T}{\partial \mathbf{v}} \frac{\partial \mathbf{q}}{\partial \mathbf{v}} = \frac{\partial S_q}{\partial \mathbf{v}} \frac{\partial \mathbf{q}}{\partial \mathbf{v}} = S_{vv} \quad (3.39)$$

$$S_{vv} = \text{Diag} \left[\frac{R}{\rho}, \frac{\rho}{T}, \frac{\rho}{T}, \frac{\rho}{T}, \frac{\rho C_v}{T^2} \right] \quad (3.40)$$

This property can alternately be demonstrated directly by grouping the primitive-conservative mappings and S_{qq} together as in,

$$D = \mathbf{q}_v^T S_{qq} \mathbf{q}_v = S_{vv} \quad (3.41)$$

The results of each approach are found to be identical, but linearization approach highlights the connection between the entropy variables and entropy as a scalar quantity.

This is equivalent to the Chu energy norm divided by a factor of temperature. This is physically consistent with the relationship between energy and thermodynamic entropy for the viscous processes. The Chu norm can be interpreted as an equivalent expression of an entropy normalization for the special case that temperature gradients are sufficiently small that Eq. 3.37 is an adequate expression of entropy, i.e, when compressibility effects are weak. The ability to arrive at a thermodynamically consistent multiple of the Chu norm by contracting against entropy also implies the existence of a family of normalizations centered on other quantities, which may be calculated through the appropriate mathematical manipulation of the entropy norm. Moreover, this sheds light on a fundamental property of the Chu norm which has been alluded to since its inception. The Chu norm is of the dimensions of energy and its derivation requires that pressure work terms be zero. From the

first law of thermodynamics, this means that the Chu norm is a heat-transfer norm. This interpretation of the Chu norm is more consistent with its relationship to the entropy norm as well. This further implies the extensibility of the normalization presented herein to cases whose entropy generation mechanisms are outside of the physics considered in this derivation, but those equivalent norms would converge to this expression of the norm under appropriate conditions. For example, a normalization derived for a two-temperature framework would be equivalent to the presented normalization in the case that the vibrational and electronic energy storage mechanisms were not excited.

A consequence of this consistency is the ability to express the Chu norm in the conservative variables. As it has been shown that the normalizations obey the relationships that govern their reference quantities, the Chu norm can be found by appropriate multiplication of S_{qq} . Another example of this property of the entropy function is demonstrated by Subbareddy and Candler [131], who showcase that a scheme which is kinetic energy consistent is also entropy conservative.

Importantly, the conservative Chu norm can't be derived through the same process by which S_{qq} was derived because total energy is one of the conservative variables. This leads to one of columns of the mapping from the conservative to the energy variables being constant, and the final dense matrix loses its dependence on energy. This represents a limitation in the process described above to convex functions. The convexity requirement was established in the discussion of mathematical entropy as well, and further demonstrates the value of entropy as a starting point for deriving matrix normalizations of all kinds.

3.4 Generalized Norm

Having demonstrated the relationship between the novel entropy normalization and the Chu energy norm for the case of a single calorically perfect ideal gas, the generalized norm may be derived. The process for deriving the general norm is

nearly identical to the ideal case, but certain quantities require more clarification. Because density appears so often in the equations, and is linked to entropy through the equation of state, it is not practical to derive a norm completely general with respect to the thermodynamic closure relationship. Instead, a version of the norm will be derived first using an ideal gas closure and then the Van-der-Waals equation of state. Other closure relationships will be left to future work, as the introduction of the two norms presented here already represent a significant expansion of the matrix normalization library available to the fluid dynamics community. The description of the Van-der-Waals permutation of the norm will also serve as a guide for the inclusion of other closures.

The fundamental definitions of thermodynamic energy and entropy are found in [121] and are expressed in terms of the partition function discussed in section 3.1, which helps bridge the gap between molecular dynamics and continuum fluid thermodynamics. The partition function describes the number of states accessible to a molecule in the system at the give microdynamic (temperature) state. Gokcen [26] describes the entropy relations used for a nonequilibrium flow using Gnoffo's model, utilizing the partition functions as described in Atkins [121]. Because these entropy expressions are functions of the independent variables of the Navier-Stokes, they provide a basis from which the entropy variables can be derived. An important point of potential contention is the treatment of the excitation partition function for the electronic excitation energy. For a single species of electronically excited gas, there are theoretically an infinite number of excited states which can be occupied by electrons approaching the ionization energy, at which the electron escapes. Because the convergence is asymptotic as the ionization energy is approached, for engineering purposes it may be sufficient to truncate the series. The exact threshold for truncation will be species specific. A detailed explanation of the behavior of the plasma is found in [132]. With the definitions of entropy, the thermodynamic state variables, the conservative and primitive flow variables, and the relationships between those

variables known or calculable, the only step required to construct the entropy normalization for these flows is calculating the matrices of derivatives and mappings.

First, the treatment of the individual constituents of multicomponent gases is addressed. Following the conventions laid out in Refs. [27] and [26], the total entropy, energy, and density are taken as the sums of the individual contributions of the constituents. Here, the relationship between partial pressures and mole fractions which gives rise to the mixing entropy is not necessary, since the total pressure (in the sense of the sum of partial pressures, not the stagnation pressure) is not used here. Instead, the entropy relationship is left as a sum of functions of the mass concentration, ρ_i , and the mixing contribution is left implicit. Each species being considered may have its own properties, such as R , and mass concentration, but locally the entire mixture is considered to have the same velocity and be at the same temperature(s). For monatomic constituents, the vibrational and rotational components of the entropy relationships are zero, and as will be seen in the norm itself, removing these components is trivial. Using 11-species air and tracking each thermal mode individually, the resulting matrix norm will be a 17×17 square matrix. The present approach has no need to directly track chemical reactions happening within the gas, since the values which make up the norm are local constants and the entropy of mixing is implicitly considered by refraining from converting the mass fractions into mixture density of absolute (as opposed to partial) pressure. Reaction dynamics are handled in fluid dynamics problems by separate models coupled to the governing equations of the flow, and the heat stored or released in these reactions allows the entropy of the reactions to be implicitly tracked as well.

Another hurdle in deriving the generalized norm is the question of taking the matrix Jacobian of the primitive variables with respect to the conservative variables. The form of the temperatures terms is left unspecified, and it is not guaranteed that the energy function is algebraically invertible in all cases. Therefore it is not immediately clear what the values of the derivatives of these terms should be. To avoid this question, rather than calculating them directly, the one-to-one mapping

between these variable sets can be utilized. Because the mapping is one-to-one, we can instead find the inverse Jacobian, the derivatives of the conservative variables with respect to the primitives, and then invert this matrix to recover the desired mapping, as in

$$\frac{\partial v}{\partial q} = \left(\frac{\partial q}{\partial v} \right)^{-1} \quad (3.42)$$

While the definition of $\frac{\partial T}{\partial s}$ is not always clear, $\frac{\partial s}{\partial T}$ is generally calculable, and can be left symbolic. This will allow for further simplification after the chain rule has been applied which eliminates the need for calculating potentially long and complex derivatives, especially if electronic contributions are considered. In presenting the generalized norm, quantities are described with the convention $X_{n,k}$ where n represents the species being considered and k represents the thermal mode being considered. Because the translational contribution is ubiquitous and here is used to consider the entropy contribution of density fluctuations, translational contributions will be denoted in the form $X_{n,tr}$ and k will take a value of 1, 2, or 3. Though not used explicitly in the description of the partition functions, C_v will be used here for consistency with the calorically perfect equilibrium norm, where $C_{v(n,k)} = \frac{\partial e_{n,k}}{\partial T_k}$.

Beginning again with the statement of entropy and differentiating with respect to the the primitive variables, then mapping to the conservatives, the entropy variables can be found. This form is very similar to the ideal gas norm, as in

$$w = S_q^T = \frac{\partial S}{\partial v} \frac{\partial v}{\partial q} \quad (3.43)$$

$$w^T = R_1 - s_1 + \frac{e_{1,tr}}{T_{tr}} + \sum_k \frac{e_{1,k}}{T_k} - \frac{||u^2||}{2T_{tr}}, \dots, R_N - s_N + \frac{e_{N,tr}}{T_{tr}} + \sum_k \frac{e_{N,k}}{T_k} - \frac{||u^2||}{2T_{tr}},$$

$$\frac{u}{T_{tr}}, \frac{v}{T_{tr}}, \frac{w}{T_{tr}}, \frac{-1}{T_{tr}}, \frac{1}{T_{tr}} - \frac{1}{T_1}, \dots, \frac{1}{T_{tr}} - \frac{1}{T_K} \quad (3.44)$$

The entropy variables calculated this way are found to agree with those calculated by Hansen and Fisher [133], who express the first entropy variable in a slightly different but equivalent form. Hansen and Fisher also do not consider electronic energy storage, but the form of these terms is shown here to be the same as other nonequilibrium quantities provide the sum of electronic energy levels is appropriately truncated. As pointed out by that author, the entropy variables do not provide any specific accounting for the chemical reaction processes taking place in the flow. Effectively, the convexity of the entropy function is dependent on the chemical reaction model also respecting the 2nd law. For CFD the chemical reaction model is generally a separate, often tightly coupled calculation from the Navier-Stokes solution process. Therefore chemical reactions are seen by the flow entropy variables as a black box whose influence is felt at each time step through changes in individual species mass fractions and the endothermic or exothermic changes in heat.

Following the same process as before, the entropy norm can be derived through the chain rule using known derivative mappings,

$$S_{qq} = \frac{\partial w}{\partial q} = \frac{\partial w}{\partial v} \frac{\partial v}{\partial q} \quad (3.45)$$

and can be expressed in terms of the primitive variables by diagonalizing using q_v . The conservative norm and other matrix identities are expressed in the appendices. The generalized S_{vv} is diagonal,

$$S_{vv} = \text{Diag} \left[\frac{R_1}{\rho_1}, \dots, \frac{R_N}{\rho_N}, \frac{\sum_n \rho_i}{T_{tr}}, \frac{\sum_n \rho_i}{T_{tr}}, \frac{\sum_n \rho_i}{T_{tr}}, \frac{\sum_n \rho_i C_{v(i,tr)}}{T_{tr}^2}, \dots, \frac{\sum_n \rho_i C_{v(i,K)}}{T_K^2} \right] \quad (3.46)$$

The ability to diagonalize the general entropy norm is significant from an implementation perspective because of how large the norm itself and the data sets it is used to analyze can be. For CFD it is common for data sets to contain flow information for hundreds of millions of cells. In examining a typical atmospheric entry case, the dense norm requires calculating and storing 153 unique values, defined locally at each

point, assuming the redundant points on the off-diagonals are stored only once. This cost adds up quickly, and the diagonal norm is just as valid while realizing an 89% reduction in data storage required.

The Van-der-Waals Gas

Before deriving the generalized norm for a Van-der-Waals gas, a few key points should be covered. The first is the issue of applicability. Obviously real-gas effects are sometimes considered in computational applications, but in general the matrix normalization is not integral to developing the representation of the flow being analyzed. For modal decompositions, the flow field is generated computationally or sampled from an experiment, and the matrix normalization comes in to play as a post-processing and analysis step. Because changing the thermodynamic closure does not change the number or type of variables required to close the system, the ideal-gas norm can be used to analyze a flow field calculated with a Van der Waals closure and vice versa. This is not necessarily good practice, but there is nothing mathematically to stop the user from doing so.

The implementation of an alternative closure is relatively straightforward by formulation of the problem. When discussing the molecular partition functions, it was stated that the translational partition function would be treated specially to separate the influence of the density perturbations from the temperature perturbations. It is also noted that the translational entropy is calculated using the Sackur-Tetrode equation. This equation describes the absolute translational entropy of an electrically unexcited molecule. Because translation is the only non-electronic mode available to monatomic species, this equation is often cited as describing the absolute entropy of monatomic species with no additional context given.

In order to develop the entropy norm for a Van der Waals gas, all that is required is to substitute the ideal gas manifestation of the Sackur-Tetrode equation for the Van

der Waals one and repeat the derivation. The Van der Waals equation of state is expressed according to

$$P = \frac{\rho RT}{1 - b\rho} - a\rho^2 \quad (3.47)$$

where a and b are gas-specific constants. The translational entropy of a Van der Waals gas is then expressed as

$$s_{tr} = R \ln\left(\frac{1}{\rho} - b\right) + \frac{3}{2} R \ln(T) + S_c \quad (3.48)$$

The generalized norm can be left otherwise unchanged, so the derivation continues as before with the entropy variables for a Van der Waals gas found to be

$$\begin{aligned} w^T = & \frac{-R_1}{(\rho_1 b_1 - 1)} - s_1 + \frac{e_{1,tr}}{T_{tr}} + \sum_k \frac{e_{1,k}}{T_k} - \frac{||u^2||}{2T_{tr}}, \dots, \frac{-R_N}{(\rho_N b_N - 1)} - \\ s_N + & \frac{e_{N,tr}}{T_{tr}} + \sum_k \frac{e_{N,k}}{T_k} - \frac{||u^2||}{2T_{tr}}, \frac{u}{T_{tr}}, \frac{v}{T_{tr}}, \frac{w}{T_{tr}}, \frac{-1}{T_{tr}}, \frac{1}{T_{tr}} - \frac{1}{T_1}, \dots, \frac{1}{T_{tr}} - \frac{1}{T_K} \end{aligned} \quad (3.49)$$

The diagonalized entropy norm for a Van der Waals gas is

$$S_{vv} = \text{Diag} \left[\frac{-R_1(2b_1\rho_1 - 1)}{\rho_1(b_1\rho_1 - 1)^2}, \dots, \frac{-R_N(2b_N\rho_N - 1)}{\rho_N(b_N\rho_N - 1)^2}, \frac{\sum_n \rho_i}{T_{tr}}, \frac{\sum_n \rho_i}{T_{tr}}, \frac{\sum_n \rho_i}{T_{tr}}, \right. \\ \left. \frac{\sum_n \rho_i C_{v(i,tr)}}{T_{tr}^2}, \dots, \frac{\sum_n \rho_i C_{v(i,K)}}{T_K^2} \right] \quad (3.50)$$

Crucially, the case where $a = b = 0$, which are the Van der Waals constants of a true ideal gas recovers the ideal gas version of the entropy norm. This builds on the findings of the relationship between the Chu and entropy norms, demonstrating that the laws of thermodynamics may be applied to matrix normalization operators to yield meaningful results. While the Van-der-Waals equation of state does not introduce any further dependency on temperature, there are alternative models which do (such as the Berthlot equation preferred by Eggers [134]). In these cases the equation must first be arranged to separate the dependence of temperature and

density, which is possible in general utilizing logarithmic relations. So long as the resultant temperature dependence is differentiable, the relations used to derive and simplify the norm will still be valid, and the derivation is otherwise the same.

3.4.1 Additional Extensions

The derivation up to this point has assumed a single temperature for each thermodynamic mode is sufficient to describe the state of the flow. However, in reality each constituent gas may have its own characteristic nonequilibrium relaxation time and therefore be described by a unique temperature. If this is the case, the last term in Eq. 3.46 would be split from a sum across constituents so that each constituent's internal thermodynamic modes are considered independently. This further increases the number of independent variables of the system and increases the size of the norm accordingly.

Chapter 4

Generalized Entropy Transport

The entropy analysis presented up to this point provides a method of calculating the entropy of a perturbation, which is useful for many analysis techniques. In constructing an L^2 norm for a reduced-order model or analyzing a perturbation inclusive of a variety of coupled dynamics, it is appropriate and necessary for the expression of magnitude to be inclusive of multiple phenomena. Because the analysis up to this point has focused primarily on the expression of entropy and the variables themselves, it does not shed light on what specific mechanisms of entropy production or transport are at play in a given system. The thorough interrogation of the specific mechanisms of entropy generation is a valuable capability in developing a thorough understanding of the state of a flow. This is particularly true for turbulence problems. Turbulence is an extremely complex and difficult problem even considering only the tamest of physics, and the increasing influence of compressibility as Mach number increases further complicates turbulence analysis.

4.1 Compressible Turbulence Analysis

Contemporary turbulence analysis focuses on the prediction of Reynolds stresses and turbulent kinetic energy. Previous sections have highlighted the shortcomings of energy methods and the connection of energy decay with entropy. In short, energy

does not actually decay, it is conserved, so methods which rely on "energy decay" of some kind must place stipulations or assumptions on the kind of energy being considered, such as kinetic energy. These methods are, by construction, vulnerable to situations in which the assumptions they make are violated and energy no longer decays as expected. By contrast, entropy does actually grow monotonically in time for all systems, and is the better candidate when such behavior is required from an analysis. Entropy analyses presented has, to this point, provided mechanisms for evaluating the entropy state of the flow, but not for calculating the entropy generation rate. The natural next step of this theoretical analysis is therefore to interrogate not only the total entropy of a flow or perturbation at a singular instance in time, but to seek a method of tabulating the generation and transport of entropy for a generalized flow.

4.2 Derivation of Entropy Transport

The combination of an entropy-centered investigation of the flow properties and a full description of the dynamic evolution of the flow will at last require direct invocation of the full, 3D Navier-Stokes equations. The statement of these equations employed here is that used by Gnoffo to develop a two-temperature model [27], though for generality a three-temperature framework is used here. Assumptions and approximations made in the development of the governing equations as stated here are discussed below. Making no assumptions as to the number of species present, taking the mixture's constituents to be described by a single temperature for each thermodynamic energy storage mechanism, and assuming that, for species for which it is applicable, rotational energy storage is in equilibrium with translational energy storage, the governing equations of a flow may be written as,

$$\frac{\partial}{\partial t}\rho_s + \frac{\partial}{\partial x_j}\rho u_j = \frac{\partial}{\partial x_j}(\rho D_s \frac{\partial}{\partial x_j}y_s) + \dot{w}_s \quad (4.1)$$

$$\frac{\partial}{\partial t}\rho u_i + \frac{\partial}{\partial x_j}\rho u_i u_j = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad (4.2)$$

$$\begin{aligned} \frac{\partial}{\partial t}\rho e_v + \frac{\partial}{\partial x_j}\rho e_v u_j &= \frac{\partial}{\partial x_j} \left(\eta_v \frac{\partial T_v}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho \sum_{all} h_{v,s} D_s \frac{\partial y_s}{\partial x_j} \right) + \\ &\sum_{mol} \rho_s \frac{e_{v,s}^* - e_{v,s}}{< \tau_s >} + \sum_{mol} \rho_s \frac{e_{v,s}^{**} - e_{v,s}}{< \tau_{e,s} >} + \sum_{mol} \dot{w}_s \hat{D}_s \end{aligned} \quad (4.3)$$

$$\begin{aligned} \frac{\partial}{\partial t}\rho e_e + \frac{\partial}{\partial x_j}((\rho e_e + p_e)u_j) &= u_j \frac{\partial p_e}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\eta_e \frac{\partial T_e}{\partial x_j} \right) + \\ \frac{\partial}{\partial x_j} \left(\rho \sum_{all} h_{e,s} D_s \frac{\partial y_s}{\partial x_j} \right) &+ 3\rho_e \bar{R}(T - T_e) \sum_{heavy} \frac{\nu_{es}}{M_s} - \sum_{ion} \dot{n}_{e,s} \hat{I}_s \\ &- \sum_{mol} \rho_s \frac{(e_{v,s}^{**} - e_{v,s})}{< \tau_{es} >} - Q_{rad} \end{aligned} \quad (4.4)$$

$$\begin{aligned} \frac{\partial}{\partial t}\rho E + \frac{\partial}{\partial x_j}\rho H u_j &= \frac{\partial}{\partial x_j} \left(\eta \frac{\partial T}{\partial x_j} + \eta_v \frac{\partial T_v}{\partial x_j} + \eta_e \frac{\partial T_e}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho \sum_{all} h_s D_s \frac{\partial y_s}{\partial x_j} \right) \\ &+ \frac{\partial}{\partial x_j} \left(u_i \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} u_i \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) - Q_{rad} \end{aligned} \quad (4.5)$$

In these equations, D_s is the diffusion coefficient of the species s , y_s is the mole fraction of the species, $\dot{w}_s$ is the mass production rate of the species, ν is the conduction coefficient of the species for the thermodynamic mode specified by the described subscript, $\hat{D}_s$ is the characteristic vibrational energy of the species being created, $e_{v,s}^*$

is the vibrational energy of the species evaluated at T , $e_{v,s}^{**}$ is the vibrational energy evaluated at T_e , $\langle \tau_s \rangle$ is the translational-vibrational relaxation time of the species, $\langle \tau_{es} \rangle$ is the electronic-vibrational relaxation time of the species, η_{es} is the collision frequency between electrons and the species, $\dot{n}_{e,s}$ is the molar rate of production of the species by electron impact ionization, $\hat{I}_s$ is the first ionization potential of the species, Q_{rad} is the radiative energy transfer, and quantities with the subscript $_e$ describe the properties of free electrons. Parameters associated with electron energy transfer, radiation, and the calculation of the relaxation and conduction parameters for the nonequilibrium quantities may be calculated using separate models and relations. These parameters will be discussed as they become important to the overall entropy calculation.

4.3 Entropy Budget of the Generalized Navier-Stokes

The right hand side of the conservative Navier-Stokes describes the factors which influence the evolution of the conservative variables through the flow field. Recalling that the entropy variables map changes in total entropy to changes in the conservative variables, the Navier-Stokes presents an opportunity describe the mechanisms of entropy generation in more detail. Once again taking advantage of the chain rule, an expression for the material derivative of entropy can be obtained. Keeping in mind that $w = S_q = \frac{\partial S}{\partial q}$, the material derivative of entropy can be expressed as,

$$\frac{\partial S}{\partial t} + \nabla \cdot (\mathbf{u}S) = \frac{\partial S}{\partial q} \left(\frac{\partial q}{\partial t} + \nabla \cdot (\mathbf{u}q) \right) \quad (4.6)$$

which can be directly equated to the inner product of the entropy variables with the righthand side terms of the Navier-Stokes. Because entropy is a scalar quantity, this

takes the form of a vector inner product, and all of the terms are summed. After appropriate simplification, the resulting inner product is found to be,

$$\begin{aligned}
\frac{\partial S}{\partial t} + \nabla \cdot (\mathbf{u}S) = & \underbrace{\sum_{all} \left((-s_s - \frac{u_i u_i}{2T}) \left(\frac{\partial}{\partial x_j} (\rho D_s \frac{\partial}{\partial x_j} y_s) + \dot{w}_s \right) + \left(\frac{h_{tr}}{T} + \frac{h_v}{T_v} + \frac{h_e}{T_e} \right) \dot{w}_s \right)}_1 \\
& - \underbrace{\frac{\rho}{T} \frac{\partial}{\partial x_j} \left(\sum_{all} h_{tr,s} D_s \frac{\partial y_s}{\partial x_j} \right) - \frac{\rho}{T_v} \frac{\partial}{\partial x_j} \left(\sum_{all} h_{v,s} D_s \frac{\partial y_s}{\partial x_j} \right) - \frac{\rho}{T_e} \frac{\partial}{\partial x_j} \left(\sum_{all} h_{e,s} D_s \frac{\partial y_s}{\partial x_j} \right)}_2 \\
& + \underbrace{\frac{Q_{rad}}{T_e}}_3 + \underbrace{\left(\frac{1}{T} - \frac{1}{T_v} \right) \left(\sum_{mol} \rho_s \frac{e_{v,s}^* - e_{v,s}}{\langle \tau_s \rangle} \right)}_4 + \underbrace{\left(\frac{1}{T_e} - \frac{1}{T_v} \right) \left(\sum_{mol} \rho_s \frac{e_{v,s}^{**} - e_{v,s}}{\langle \tau_{e,s} \rangle} \right)}_5 \\
& - \underbrace{\frac{1}{T} \frac{\partial}{\partial x_j} \left(\eta \frac{\partial T}{\partial x_j} \right) - \frac{1}{T_v} \frac{\partial}{\partial x_j} \left(\eta_v \frac{\partial T_v}{\partial x_j} \right) - \frac{1}{T_e} \frac{\partial}{\partial x_j} \left(\eta_e \frac{\partial T_e}{\partial x_j} \right)}_6 - \underbrace{\frac{1}{T} \left(\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \frac{\partial u_i}{\partial x_j}}_7 \\
& + \underbrace{\left(\frac{1}{T} - \frac{1}{T_v} \right) \left(\sum_{mol} \dot{w}_s \hat{D}_s \right)}_8 - \underbrace{3 \frac{(T - T_e)^2}{TT_e} \rho_e \sum_{heavy} (\nu_{e,s} R_s)}_9 - \underbrace{\left(\frac{1}{T} - \frac{1}{T_e} \right) \sum_{ion} \dot{n}_{e,s} \hat{I}_s}_{10}
\end{aligned} \tag{4.7}$$

which is a complete description of the evolution of the entropy of the flow. The subscripts used here are as follows: *all* refers to all species including electrons in the mixture, *mol* refers to al species consisting of two or more atoms, *heavy* refers to all species excluding free electrons, and *ion* refers to ionized species. In the calculation of this inner product, the pressure and total energy terms are rearranged such that the transport terms on the lefthand side are exclusively in terms of the conservative variables. This is required for for the entropy variables to correctly map entropy to the conservative variables, and also provides a convenient simplification of the pressure and viscous work terms from the momentum and total energy equations. Through this process it is found that pressure work cancels from both sides of the entropy transport equation, as reversible work does not produce entropy.

The terms of this equation are grouped according to the entropy mechanism they represent. Groups 1 and 2 come from the species continuity equations and represents the entropy "carried with" molecules of a species as they dissociate or recombine into a different species or as molecules of a species diffuse within the flow. These

mechanisms describe the entropy generated by non-conservative transport of mass, since the energy associated with those molecules must still be conserved.

Group 3 is the entropy of heat transfer via radiation, the form of which Gnoffo does not specify. It should be highlighted that the entropy from radiation is found to depend solely on the electronic temperature, which is consistent with radiation's mechanism of action. Radiation heat transfer occurs when excited electrons move up or down quantum energy levels, and the energy differential between the quantum states is emitted as an electron. Impinging radiation is absorbed by the inverse process.

Group 4 is the entropy generated by the relaxation between vibrational and translational-rotational energy, which grows as the discrepancy between the energy saturation of the two modes increases. This entropy exchange is driven by collisions between molecules. Group 5 is similarly the entropy generation by the relaxation of vibrational and electronic energy. Regardless of the nonequilibrium state (which temperature is higher or lower than the other) the entropy generation by nonequilibrium has the same sign. This means that any thermal nonequilibrium, regardless of its specifics, results in entropy generation. In this way, nonequilibrium acts as an internal temperature gradient down which heat is irreversibly "conducted".

Group 6 is the entropy arising from heat conduction in each energy storage mode. As with radiation, the conduction of each mode is dependent only on the temperature associated with the mode in question. This finding is physically intuitive, and guarantees that for a calorically imperfect equilibrium gas (for which only one temperature need be considered but C_v and C_p are not constant) the conduction terms will collapse to a single term whose conduction coefficient η is the sum of all three constituent modes.

Group 7 is the entropy arising from viscous dissipation. This term is identical to its calorically perfect, equilibrium counterpart. Physically, this demonstrates the energy cascade which can result in thermal nonequilibrium in flows without energy flux through the boundary. Viscosity-mediated dissipation irreversibly transforms

kinetic energy into translational thermal energy, leaving the other energy modes under-excited and leading to energy relaxation.

Group 8 is the entropy generation from molecular depletion or production because species which are incapable of storing vibrational energy may recombine to form species which can, and species which can store energy this way may dissociate into species which cannot. This process still obeys net conservation of energy, but that energy must be transformed to another form through the dissociation or recombination process. The specifics of this mechanism, like other chemical reactions, must be handled at the level of the reaction model.

Group 9 is the entropy generated by the collisions between electrons and heavier species, which is also found to scale with the nonequilibrium. This is because these collisions are a mechanism of energy transfer between the two modes, and if the flow is in thermal equilibrium the net transfer is nil.

Group 10 is the entropy associated with energy loss resulting from electron impact ionization for each species. This scales with nonequilibrium for similar reasons to group 9.

An immediate takeaway from this analysis is the rigorous demonstration that nonequilibrium thermodynamics and the consideration of free electron species introduce multiple mechanisms of entropy generation that grow as the importance of these nonequilibrium effects increases. It also shows that the transfer of energy from one internal mode to another is not necessarily isentropic. In fact, it is observed that for the relaxation terms, the monotonicity of the internal energy modes with respect to temperature guarantee that the entropy generation of thermal nonequilibrium is negative. Remembering that the entropy variables are based in mathematical entropy, which is by convention the negative of physical entropy, it is seen that the thermal relaxation of any kind increases the entropy of the gas. Many of these terms rely on species-specific constants or parameters which are themselves functions of the thermodynamic state of the flow. It should also be noted that, while electron pressure is grouped with the rest of the pressure terms, it includes the effective pressure exerted

on electrons by electrostatic repulsion. The electron pressure is calculated using the chosen thermodynamic closure with the electronic temperature rather than the translational-rotational temperature. Nearly all of these parameters are calculated using a thermodynamic or chemical model, meaning that there are many possible specific implementations which could be used to calculate the entropy, and one does not necessarily need to use the same one to analyze data as was used to develop it. Moreover, this description of entropy can provide detailed information about specific processes if one wishes to analyze only their contributions. Lastly, the inclusion of a pressure term means that the closure must be specified and the choice of closure will influence the calculated entropy.

4.3.1 Comparison with Bejan's Entropy Generation

Bejan's work in entropy analysis provided a relationship for the entropy generation in a flow [135], which has seen widespread use and success [136]. Bejan focuses on two mechanisms of entropy generation, viscous dissipation and thermal dissipation. Using nomenclature conventions consistent with its original presentation, Bejan's entropy generation is expressed as

$$S' = \frac{\partial S}{\partial t} + \nabla \cdot (\mathbf{u}S) + \nabla \cdot \left(\frac{q}{T} \right) = \left(\frac{\Phi\mu}{T} \right) + \frac{\eta}{T^2} \left(\frac{\partial T}{\partial x} \right)^2 \quad (4.8)$$

where Φ is the viscous dissipation tensor and q is the local heat flux, not the conservative variable set. The viscous dissipation calculated by Bejan is seen to be identical to the term in group 8 of Eq. 4.7 remembering the reversed sign conventions of the analyses. The heat transfer term, however, requires more investigation. Bejan's derivation allows for arbitrary modes of thermal dissipation through the generalized heat transfer term in the definition of the entropy generation. Unlike Bejan, however, the relationship described here does not include a heat flux term in the definition

of the entropy transport, so that term must be moved to the righthand side for comparison. Assuming that heat conduction is the only mode of the generalized heat transfer in Bejan's relationship and a constant heat transfer coefficient (as Bejan's analyses do), the total entropy produced by conduction in Bejan's expression is

$$S'_{cond} = \frac{\eta}{T^2} \left(\frac{\partial T}{\partial x} \right)^2 + \frac{\partial}{\partial x} \left(\frac{k}{T} \frac{\partial T}{\partial x} \right) \quad (4.9)$$

the second term of which can be expanded via integration by parts and the chain rule, assuming a spatially-varying temperature field, yielding the relationship

$$S'_{cond} = \frac{\eta}{T^2} \left(\frac{\partial T}{\partial x} \right)^2 + \frac{\partial}{\partial x} \left(\frac{\eta}{T} \frac{\partial T}{\partial x} \right) = \frac{\eta}{T^2} \left(\frac{\partial T}{\partial x} \right)^2 + \frac{\eta}{T} \frac{\partial^2 T}{\partial x^2} - \frac{\eta}{T^2} \left(\frac{\partial T}{\partial x} \right)^2 \quad (4.10)$$

or expressed another way,

$$S'_{cond} = \frac{1}{T} \frac{\partial}{\partial x} \left(\eta \frac{\partial T}{\partial x} \right) \quad (4.11)$$

Accounting for the reversed sign conventions between the two methods, the two expressions are again identical. Coincidence with Bejan's method, which is widely accepted in literature and formulated directly from thermodynamic analysis rather than a mathematical intermediary, provides greater confidence in the predictions made by the calculations here that extend beyond the physics Bejan considered in his original derivation.

4.3.2 Simplification of the Generalized Entropy Budget

As was done with the entropy normalization, it is informative to examine the behavior of the entropy expression as the assumptions of a thermally and calorically perfect

single species in thermal equilibrium are re-introduced. It is immediately clear that enforcing the assumption of thermal equilibrium will eliminate many of the terms of the equation. Specifically, the correction terms, which account for the mis-prediction of pressure and diffusion of enthalpy are eliminated, as are the relaxation terms. This makes sense as relaxation processes don't occur under equilibrium and the total internal enthalpy and pressure terms are fully descriptive if the flow is in thermal equilibrium. The electron impact and ionization terms are also removed, as under an equilibrium flow there is no net energy transfer by collision, ionization, or dissociation. The continuity terms are still present, however. The assumption of thermal perfection has no impact besides to dictate the means of calculating the pressure term. The assumption of caloric perfection eliminates all vibrational and electronic terms, as these mechanisms account for caloric imperfection in thermal equilibrium flows. Radiation is often neglected in aerodynamics problems as well. The assumption of a single species removes all diffusion and dissociation/recombination terms, including the continuity terms.

For the conventional compressible Navier-Stokes equations, the only entropy generation terms are the pressure work, the conduction term, and the viscous dissipation term. It was noted in the derivation of the entropy norm that, for the case of an incompressible flow, the only mechanism of mathematical entropy generation available is viscous dissipation. Because an incompressible flow's thermodynamics are decoupled from its kinematics, conduction is not considered as a mechanism of entropy generation. Therefore, the only remaining terms are the pressure work and the viscous dissipation. Incompressible gases do no net work on their surroundings leaving only the viscous dissipation term. This is consistent with the theoretical analysis conducted in the entropy norm's derivation, and further demonstrates the divergence of entropy and kinetic energy dissipation as compressibility and other physics enter consideration.

4.3.3 Entropy Production of Turbulence

Equation 4.7 captures the evolution of the entropy in a flow in a total sense. This is a useful starting point for evaluating the entropy generation of turbulence and for the characterization and prediction of turbulent flows at highly-compressible conditions, including cases with nonequilibrium thermochemical effects. In order to evaluate the entropy of turbulence, it is necessary to separate the scales of the turbulence from the rest of the flow. The space and time scales of turbulence are much smaller than those characteristic of "bulk" flow features, and the fluctuations in the flow variables associated with turbulence are often much smaller than the total values of the variables. This contrast between the turbulent and bulk flow scales allows the total entropy change to be re-written in a way to separate these scales from one another. In order to do this, the equations are projected into a mean and perturbation space, where the mean flow is taken to act on a much longer time scale than turbulent fluctuations, and as such be constant with respect to them. For compressible flows, it is advantageous to use density-weighted (Favre) averaging to define the mean flow. The density-weighted average is calculated according to,

$$\tilde{\xi} \equiv \frac{\int_t \rho(t) \xi(t) dt}{\int_t \rho(t) dt} \quad (4.12)$$

with

$$\xi = \tilde{\xi} + \xi'' \quad (4.13)$$

whereas the Reynolds averaging scheme familiar from lower speed aerodynamic analysis is,

$$\bar{\xi} \equiv \frac{\int_{\tau} \xi(t) dt}{t} \quad (4.14)$$

with

$$\xi = \bar{\xi} + \xi' \quad (4.15)$$

Any flow quantity can be expanded using either scheme, and the two may be used together when appropriate. In most analyses for compressible flows the conservative variables are averaged, which is in practice Favre averaging of the primitive quantities. Density and pressure are still Reynolds averaged because these terms are the same in the conservative and primitive expressions of a flow. Equation 4.7 can be projected onto a turbulent disturbance field by substituting in the appropriate decomposition and then expanding the terms. The resulting relationship can then be averaged again and a governing differential equation for the evolution of the mean flow including the contributions from the perturbations can be recovered. Many quantities in Eq. 4.7 depend on species density rather than mixture density, and for these Favre averaging is actually more unwieldy even though compressibility is considered in these terms. The result of this analysis is somewhat lengthy, and so each term will be considered in isolation. The identities used to simplify these expressions are available in the literature. The fully expanded projected equations are presented in Appendix B, and any simplifications are discussed there on a term-by-term basis.

Chapter 5

Non-Modal Growth of Instabilities

Data Source Statement

The analysis of calorically perfect, thermal equilibrium compressible boundary layers was originally conducted for a submission to the Journal of Theoretical and Computational Fluid Dynamics which is currently under review for publication, and has been adapted for inclusion here.

5.1 Compressible Boundary Layers

The method for generating a self-similar boundary layer was that of Klunker and McLean [137], also used by Bitter and Shepherd [98], [21] for non-modal growth analysis. The former apply this method to calorically perfect flows in thermal equilibrium, and the latter add the effects of thermal nonequilibrium.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (5.1)$$

$$\rho \frac{Du}{Dt} + \nabla P = \nabla \tau \quad (5.2)$$

$$\rho \frac{Dh_{tr}}{Dt} + \frac{DP}{Dt} = -\nabla(q_{tr}) + \Phi \quad (5.3)$$

Here, the heat flux is expressed in terms of the temperature gradient, as in

$$q_{tr} = -k_{tr} \nabla T \quad (5.4)$$

By boundary layer scaling arguments and the assumption of no pressure gradient, the boundary layer equations can be derived. Here, the equations are written in terms of the similarity parameter,

$$\eta = y \sqrt{\frac{U_e}{\nu_e x}} \quad (5.5)$$

The similarity coordinate system allows for the system to be solved on a fixed domain size. Re-writing the equations in terms of the similarity variable yields

$$\rho u x \frac{\partial u}{\partial x} - \frac{\partial}{\partial \eta} \left(\mu \frac{\partial u}{\partial \eta} \right) - \frac{\partial u}{\partial \eta} \left(g + 2x \frac{\partial g}{\partial x} \right) = 0 \quad (5.6)$$

$$\rho u x \frac{\partial T}{\partial x} - \frac{1}{\sigma_e} \frac{\partial}{\partial \eta} \left(k \frac{\partial T}{\partial \eta} \right) - (\gamma_e - 1) M^2 \mu \left(\frac{\partial u}{\partial \eta} \right)^2 - \frac{\partial T}{\partial \eta} \left(g + 2x \frac{\partial g}{\partial x} \right) = 0 \quad (5.7)$$

where

$$g = \frac{1}{2} \int_0^\eta (\rho u) d\eta' \quad (5.8)$$

For this method, the similarity variable η is normalized only by the Reynolds number and the physical position of the boundary layer, which moves the dependence on the integral over the boundary layer into the profile calculation process. The x-direction derivatives may then be neglected, yielding

$$g \frac{\partial u}{\partial \eta} + \frac{\partial}{\partial \eta} \left(\mu \frac{\partial u}{\partial \eta} \right) = 0 \quad (5.9)$$

$$g \frac{\partial T}{\partial \eta} + \frac{1}{\sigma_e} \frac{\partial}{\partial \eta} \left(k \frac{\partial T}{\partial \eta} \right) = -(\gamma_e - 1) M^2 \mu \left(\frac{\partial u}{\partial \eta} \right)^2 \quad (5.10)$$

which is solved via the method of successive approximations of Klunker and Mclean [137]. The full method is described in the associated references, but the application

of the the method to the velocity terms is given for demonstration purposes. Eq. 5.9 can be re-written in a form which facilitates the use of an integrating factor,

$$\frac{\partial}{\partial \eta} \left(\mu \frac{\partial u}{\partial \eta} \right) + \frac{g}{\mu} \left(\mu \frac{\partial u}{\partial \eta} \right) = 0 \quad (5.11)$$

which can be simplified with the integrating factor,

$$\Phi = e^{\int_0^\eta \frac{g}{\mu} d\eta'} \quad (5.12)$$

which can itself be found via numerical integration, and allows the equation to be expressed as

$$\frac{\partial}{\partial \eta} \left(\frac{1}{\Phi} \frac{\partial u}{\partial \eta} \right) = 0 \quad (5.13)$$

which can again be found via numerical integration given an appropriate initial condition, in this case the no-slip wall condition. Starting with an initial approximation of the solution, the correct profile is found by repeatedly re-calculating the profile via numerical integration from the wall until the solution converges. In this case, the convergence criterion is an L^2 residual norm less than 10^{-12} .

5.2 Non-Modal Growth Calculations

The prediction of the non-modal growth of instabilities is an important application of matrix normalizations for compressible flows. It is also a valuable analysis tool when investigating a novel normalization scheme because the computational cost of performing such an analysis is usually significantly lower than other applications of norms, such as POD. The goal of this phase of stability analysis is two-fold. First, it seeks to validate the expectations of the relationship between the Chu and entropy norms at low Mach number. The second goal is to evaluate the extent of the divergence between the predictions made by each method and at what characteristic Mach numbers those changes occur.

5.2.1 Linear Stability

Stability analysis was performed from linear stability theory on thermal equilibrium boundary layers following the procedure of Hanifi et al. [57]. As is common in stability analysis, the linear stability equations are re-written with perturbations in the streamwise and spanwise directions presumed to be periodic in space and time. This allows the derivative operators to be expressed algebraically, as the derivative of a periodic function always assumes the same known form. These derivatives are used to construct a linear evolution matrix operator and the growth of perturbations can be found by tracking some representative quantity. Hanifi used the Chu norm to calculate perturbation energy for their analysis, and the entropy norm is employed alongside the Chu norm here. In the construction of the matrix eigenvalue problem which arises from the spectral collocation method used here, Hanifi replaces the rows of the conservation equation matrix corresponding to the boundaries with multiples of A . This was found to produce some spurious eigenmodes but does not meaningfully impact the solution at high Mach numbers. At lower Mach numbers spectra trimming can be employed to counteract this.

This analysis utilized quantities defined on Chebyshev collocation points. This distribution was chosen to maintain spectral accuracy through the differentiation. The base flow profiles themselves were calculated on a very dense uniform mesh, which was interpolated onto the Chebyshev basis. The Malik mapping [138] of the Chebyshev collocation points was used to cluster points between the wall and the boundary layer edge, δ_{99} , which greatly reduced the number of collocation points required to converge the non-modal growth calculation. Examples of thermal equilibrium boundary layer profiles calculated using this method are shown in Fig. 5.1, which shows both an adiabatic wall and isothermal wall profile.

Non-modal growth analysis examines the growth or decay in time of imposed disturbances using stability theory. This is done by imposing small perturbations whose properties are known, and examining the response through the eigenmodes of

the system. The disturbances imposed on the base flow for this analysis are of the form

$$\mathbf{q}(x, y, z, t) = \widehat{\mathbf{q}}(y, t)e^{i(\alpha x + \beta z)} \quad (5.14)$$

and evolve in time according to

$$\frac{\partial}{\partial t}\widehat{\mathbf{q}}(y, t) = -i\mathcal{L}\widehat{\mathbf{q}}(y, t) \quad (5.15)$$

The assumption of exponential time dependence transforms the initial value problem from into an eigenvalue problem, as in

$$\widehat{\mathbf{q}}(y, t) = \widetilde{\mathbf{q}}(y)e^{-i\omega t} \quad (5.16)$$

which leads to the eigenvalue problem

$$\mathcal{L}\widetilde{\mathbf{q}} = \omega\widetilde{\mathbf{q}} \quad (5.17)$$

The resulting eigenvectors of the linear system are non-normal. In the context of non-modal analysis, $\mathbf{q}$ denotes perturbations of the flow quantities around the provided base state.

The role of the matrix normalization in this analysis is to unify the dimensionality of the flow variables to make sure that the analysis fairly considers all potential forms of dynamic behavior. The definition of the non-modal growth (or gain) utilized here is given by

$$G(t) = G(\alpha, \beta, R, t) = \max \frac{\|\widehat{q}(t)\|_{\mathcal{M}}^2}{\|\widehat{q}(0)\|_{\mathcal{M}}^2} = \|F\Delta F^{-1}\|_2^2 \quad (5.18)$$

where

$$\Delta = \text{diag}(e^{-it\omega_1}, \dots, e^{-it\omega_K}), \quad A = F^H F, \quad A = \int_0^\infty \widetilde{q}_k^H \widetilde{q}_l dy \quad (5.19)$$

where $||\hat{q}(t)||_{\mathcal{M}}^2$ is the weighted L^2 norm of the vector of perturbations. The amplification or non-modal growth is the ratio of the magnitude of the normalized quantity in the flow at some time to the initial magnitude of the perturbation.

Because the Chu norm was developed as a tool for stability analysis of compressible flows, it is a natural first step in comparing the Chu norm to the novel entropy norm. The energy of the perturbation is generally interpreted as the mean strength of the perturbation, so if the perturbation energy rises in time, the perturbation get stronger and the flow is unstable [99]. The perturbation entropy can similarly be interpreted as the irreversible losses incurred by the perturbation, and if these losses continue to accumulate at an accelerating rate, the flow is similarly unstable. Because entropy and energy are closely related, it should not be expected that the two norms will predict radically different non-modal behaviors. From an applied standpoint, the features of interest for the calorically perfect, equilibrium gas non-modal growth analysis are the relative emphasis each norm tends to place on perturbations of different kinds. This may be manifested in the relative sensitivity to temperature gradients in the flow, which may be examined by applying different boundary conditions. More fundamentally, this analysis may be used to evaluate the predictions made in theoretical analysis of the coincidence of the two norms at low Mach number.

5.3 Results

The non-modal growth analysis of the calorically perfect, thermal equilibrium, self-similar boundary layer were compared to the results of Hanifi et al. [57]. Hanifi used the Chu norm to analyze the growth of instabilities, and so are a useful validation of the results gathered here. The first such validation is the evaluation of the Reynolds number scaling of the amplification profiles for otherwise consistent conditions. As shown in Fig. 5.2, the profiles are shown to collapse to an identical profile with the appropriate Reynolds number scaling, which is consistent with Hanifi's results. This is a property first identified by Gustavsson [139] and Reddy and Henningson [140] for

lower Mach numbers, and states that, all other things being equal, amplification, G , will vary with Re^2 and t^{max} , the time at which maximum amplification occurs, varies linearly with Re .

In their analysis, Hanifi examines the impact of portions of the eigenspectra on the predicted growth of instabilities to identify which eigenvalues drive non-modal growth. This analysis included the presentation of non-modal growth profiles at specific conditions. These cases are used to validate the present results. The first validation case is shown in Fig. 5.3, and examines the non-modal growth of a self-similar profile at a Reynolds number of 300, a Mach number of 2.5, a total temperature of 333 K, and Fourier components $\alpha = 0.0$ and $\beta = 0.1$. Here, α and β are the streamwise and spanwise wave numbers of the initial perturbation shape, and are prescribed for each analysis. The second validation cases is for an oblique disturbance with Fourier components $\alpha = 0.06$ and $\beta = 0.1$. The self-similar boundary layer profiles into which the disturbance is seeded is Mach 2.5 with a Reynolds number of 3000, and is shown in Fig. 5.4. These figures show sufficiently close agreement with the results of Hanifi for this analysis to be taken as an accurate predictor of non-modal growth of instabilities. From this point, the analysis using the entropy norm can continue and be compared to results calculated using the Chu norm.

Hanifi et al [57] evaluated the convergence of their analysis by evaluating the convergence of the non-modal growth profiles predicted by it. Hanifi used 100 Chebyshev collocation points, which was found in their analysis to be sufficient to converge the profiles. Examining the largest eigenvalue demonstrates that the solution for the analysis is not converged with 100 collocation points. Eigenvalue convergence was evaluated using a Mach 1, cold-wall case at a Reynolds number of 3000. Despite this case having less severe temperature and velocity gradients than many of the other cases used for analysis, it was found to require finer resolution for convergence than cases at higher Mach number or with different wall conditions. This included requiring more points for convergence than cold, hot, or adiabatic wall cases examined up to Mach 20. Because this profile was more difficult to converge

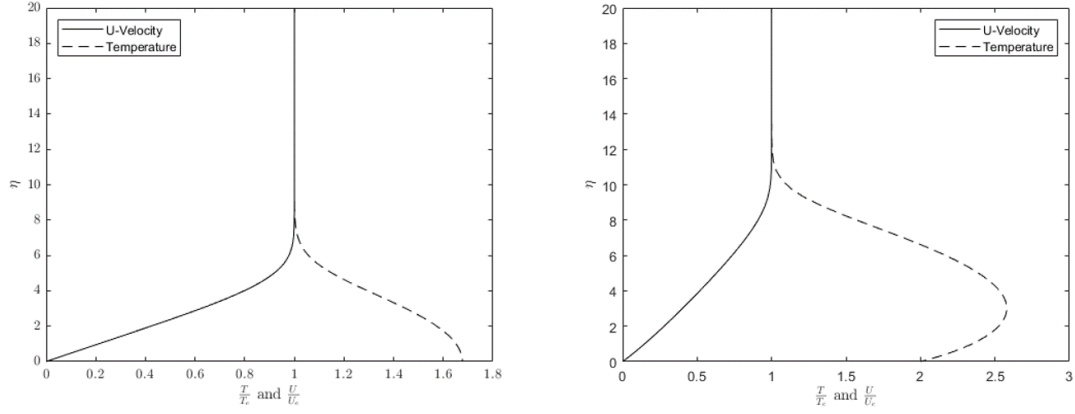


Figure 5.1: Boundary layer profiles with different Mach numbers and wall boundary conditions. The profile on the left is calculated with an adiabatic wall boundary condition at Mach 2, and the profile on the right is calculated with an isothermal wall boundary condition at Mach 5

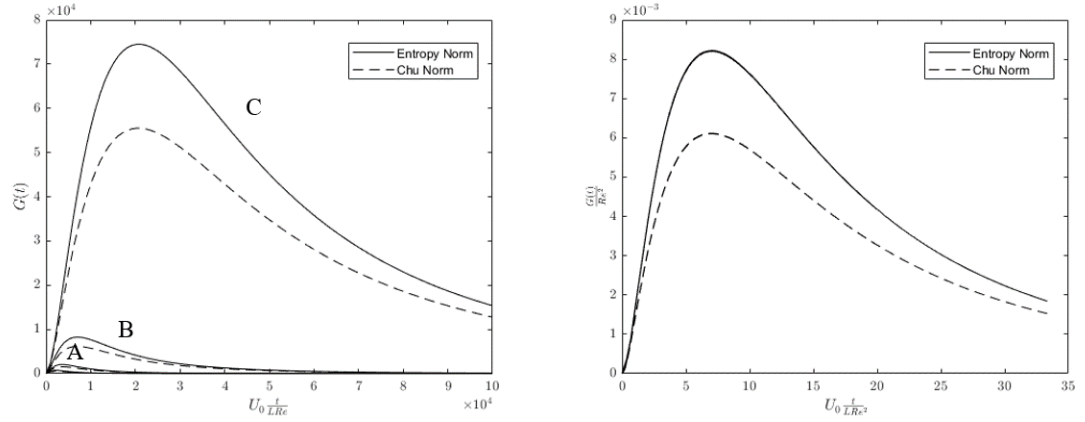


Figure 5.2: Amplification in boundary layers with the same edge Mach number with Reynolds numbers of A) 500, B) 1000, and C) 3000 (left) is shown to collapse to a single profile when normalized by Reynolds Number (right)

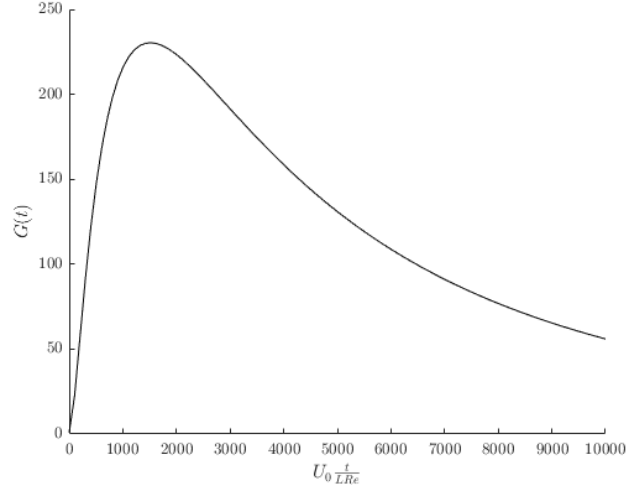


Figure 5.3: Amplification in energy in a Mach 2.5 boundary layer at a Reynolds number of 300 with wave number components $\alpha = 0.0$ and $\beta = 0.1$. This figure demonstrates agreement with Fig 5. of [57], who performed a similar analysis at the same conditions

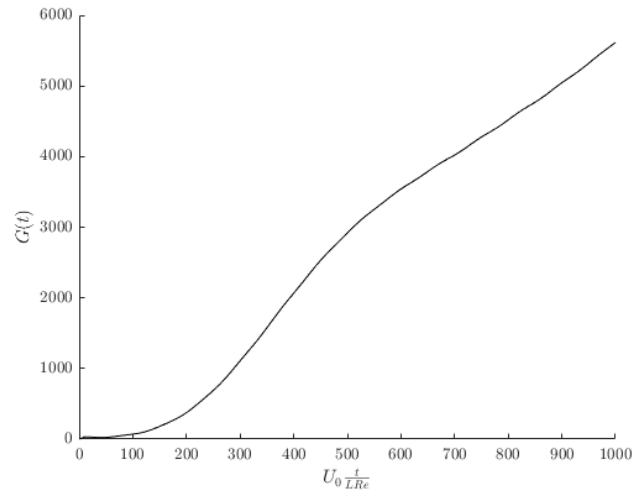


Figure 5.4: Amplification in energy in a Mach 2.5 boundary layer at a Reynolds number of 3000 with wave number components $\alpha = 0.06$ and $\beta = 0.1$. This figure demonstrates agreement with Fig 4. of [57], who performed a similar analysis at the same conditions. Spectra trimming was employed for this case

than other examined cases, it was considered an indicator for convergence of cases in general. The convergence of the largest eigenvalue for the validation cases is shown in Table 5.1.

Table 5.1: Convergence of the largest eigenvalue of the compressible self-similar boundary layer analysis with increasing Chebyshev collocation points. For simplicity, the real portion of the eigenvalue is reported

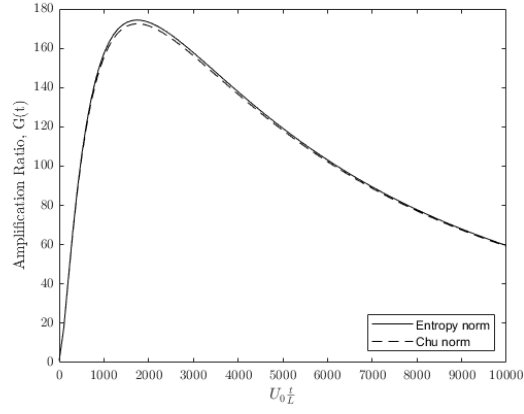
N	$ \omega_{max} $
100	0.00571571
120	0.00149721
140	$3.34659332 \times 10^{-5}$
160	$3.34659333 \times 10^{-5}$
180	$3.34659333 \times 10^{-5}$
200	$3.34659333 \times 10^{-5}$

Non-modal growth is analyzed here with 180 Chebyshev collocation points per run. This provided sufficient point density to converge the eigenvalues of the spectrum and ensured that features above the boundary layer were adequately resolved. This was paid particular attention because the Malik mapping clusters points inside of the boundary layer.

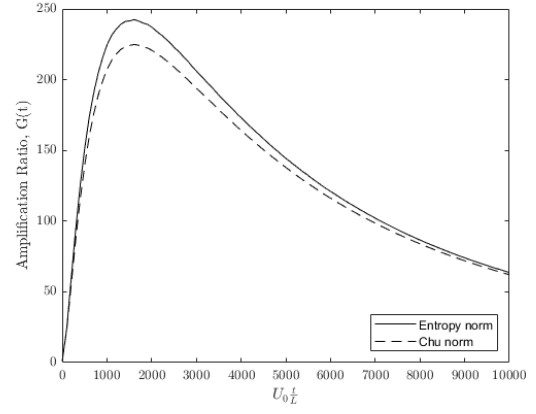
One of the chief goals of the present analysis is to validate the expected convergence of the predictions of each norm at the incompressible limit. For this application, that would mean that the amplification profiles predicted by each norm should be identical for the case where $M = 0$. The amplification over time for boundary layer profiles with the same edge and wall thermodynamic conditions but with different Mach numbers are shown in Fig. 5.5. The expected profile convergence is demonstrated here. Moreover, the divergence between the norms is shown to increase with increasing Mach number. This corresponds to an increase in the dominance of temperature gradients in the flow, and is consistent with the dependence of energy and entropy on temperature.

Another observation from these results is that the entropy norm shows the same qualitative behavior as the Chu norm for all of the Mach numbers examined here. The entropy norm demonstrates similar behavior relative to the Chu norm for the case where wall temperature changes. This analysis is shown in Fig. 6.2. The norms predict more similar profiles for the cold wall case than the hot wall case, but in both the profiles demonstrate qualitative agreement and the maximum gain appears at the same point in time. These two figures demonstrate the sensitivity of the entropy normalization to temperature gradients in the base flow.

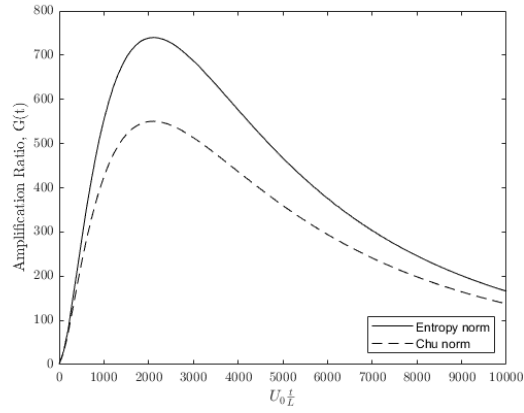
Examination of the non-modal growth profiles for various conditions is sufficient to establish the general behavior of the entropy norm relative to the Chu norm, but it is not on its own sufficient to determine the source of the differences in predicted amplifications. Therefore, it is beneficial to examine the predicted disturbances calculated using each norm. Before this, there is an important peculiarity of the non-modal growth analysis that must be discussed. As mentioned in Hanifi [57], the boundary conditions at the far field, which are required to close the linear system, are difficult to enforce. This introduces eigenvalues to the system mapped away from the domain of interest. In the perturbation shapes these manifest as noise at lower Mach numbers, so it may be desirable to trim the eigenspectrum so as to remove the influence of these spurious eigenvalues. This is particularly important when examining the temperature perturbation profiles of low-Mach number cases, where the coupling between the velocity and temperature is weak and the temperature perturbations are low in magnitude, because the noise in these profiles can dominate the non-modal behavior. Overzealous trimming of the eigenspectrum can exclude eigenvalues of interest and alter the observed amplification. Here, only the perturbation shapes calculated at Mach 3 or below use a trimmed spectrum. At higher Mach numbers, the increased coupling between the temperature and velocity perturbations suppresses noise in the temperature perturbations, eliminating the need for trimming the spectrum. The impact of spectrum trimming is shown in Fig. 5.7. As can be seen, removing the eigenvalue corresponding to the noise has a small impact



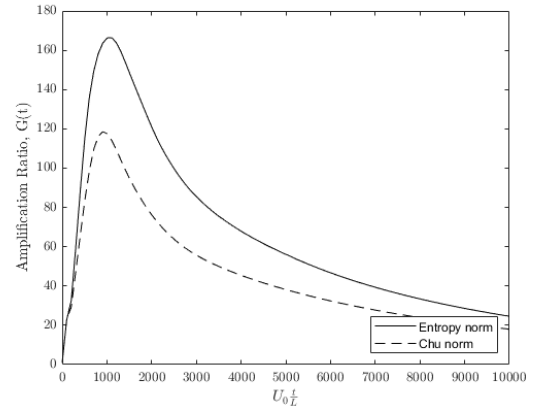
((a)) $M = 0.5$



((b)) $M = 1$



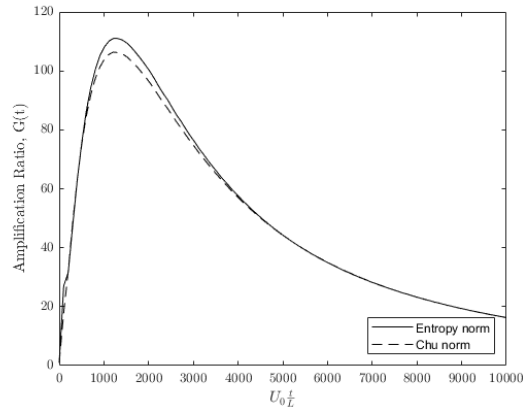
((c)) $M = 5$



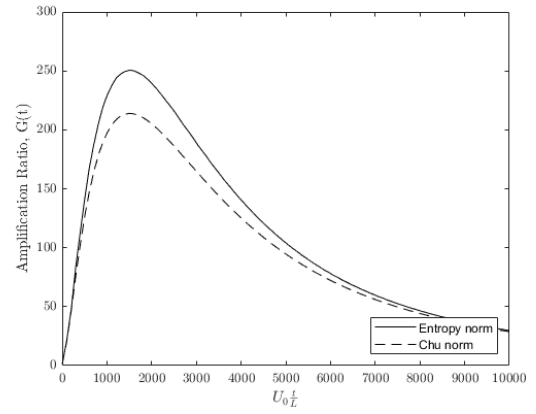
((d)) $M = 10$

Figure 5.5: Amplification as calculated by Chu and entropy normalizations for compressible self-similar boundary layer profiles showing increasing divergence as Mach number increases

on the profile near the wall, but the spectrum alteration is necessary to uncover the dominant instability shape. There is also potential for these spurious modes to obscure or suppress the dynamics which are actually of interest. This is observed in the velocity profile of the Mach 1 disturbance.



((a)) $T_w = \frac{1}{2}T_e$



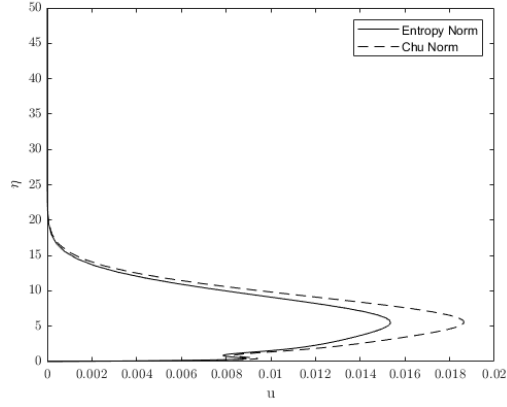
((b)) $T_w = 2T_e$

Figure 5.6: Amplification predicted by each normalization in a Mach 5, boundary layer at a Reynolds number of 300

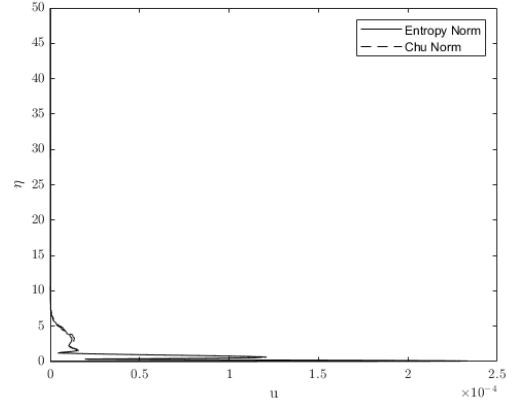
With this in mind, the shapes of the perturbations predicted by each normalization can be examined. Based on the mathematical exploration of the norm and the trends found in the amplification predicted by each norm, deviation is expected between the two for higher Mach numbers. Examining the modes themselves is aimed at shedding light on the mechanisms driving this expected disagreement. The initial and optimal disturbances for the Mach 1 boundary layer with $\alpha = 0$ and $\beta = 0.1$, an adiabatic wall, and a Reynolds number of 300 is shown in Fig. 5.8. Fig. 5.3 shows the same for Mach 5, and Fig. 5.10 for Mach 10. The critical nondimensional time was found not to change as a function of Mach number, and was approximately 1800 in each of the cases presented in these figures.

Similar to the findings of Hanifi, the primary disturbance feature seen in these figures is a streamwise vortex feature in the velocity profile. The prevalence of this feature increases with Mach number. While temperature disturbances are more amorphous, except in the Mach 1 case where temperature does not yet play a significant role in the instability. The need to ensure that all features in these profiles are adequately resolved was a major driver of the choice of 180 Chebyshev points, as the Malik mapping clusters points away from some of these features and in the boundary layer.

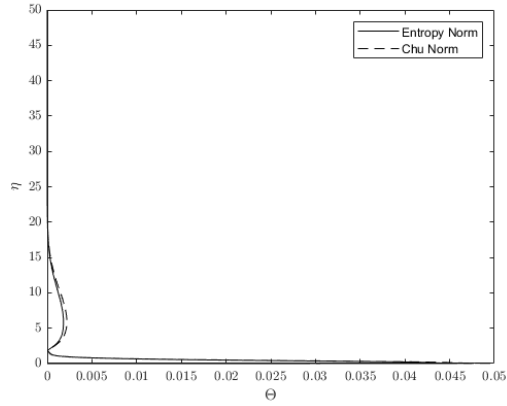
A number of behaviors expected from the mathematical analysis of the entropy norm. The first is the convergence of both the optimum inputs and outputs at low Mach numbers. At low Mach number the shapes and magnitudes of the disturbances are demonstrated to converge. It is also worth noting that, while the magnitudes of disturbances diverge with increasing Mach number for the whole domain, phenomenological differences in the mode shapes appear around Mach 5. This roughly corresponds to the onset of the hypersonic flow regime. This result is convenient, and if supported by further research could provide yet another loose definition for the onset of hypersonic flow- the point at which the stability predictions of energy and entropy demonstrate morphological divergence. Noting the different scales in these figures, it can be observed in these figures that the general magnitude of



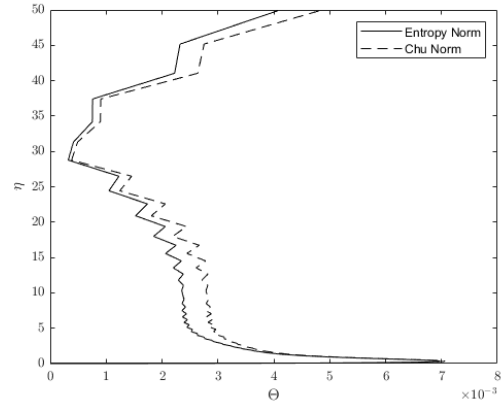
((a)) Velocity with spectra trimming



((b)) Velocity without spectra trimming

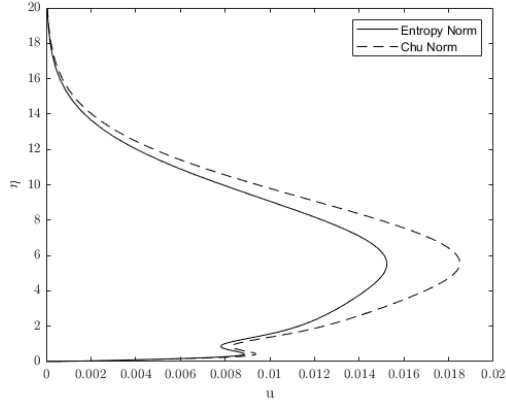


((c)) Temperature with spectra trimming

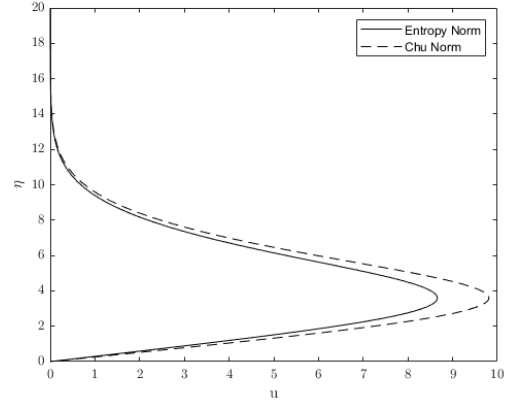


((d)) Temperature without spectra trimming

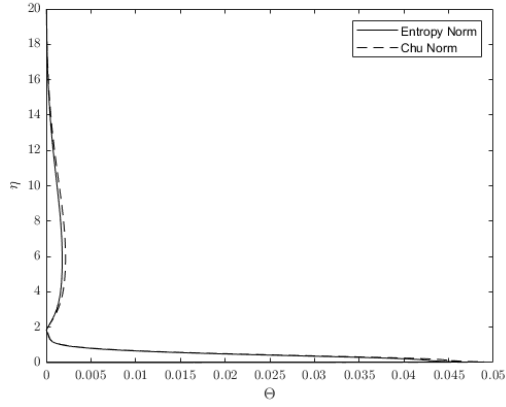
Figure 5.7: Mach 1 boundary layer instabilities with and without spectra trimming



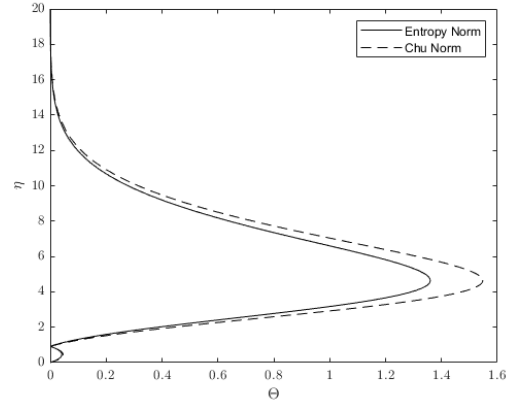
((a)) Optimal velocity input mode



((b)) Optimal velocity output mode

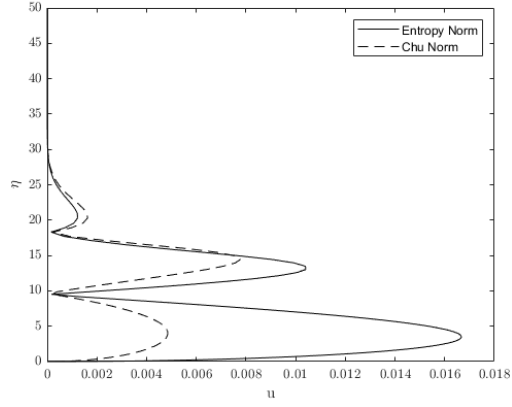


((c)) Optimal temperature input mode

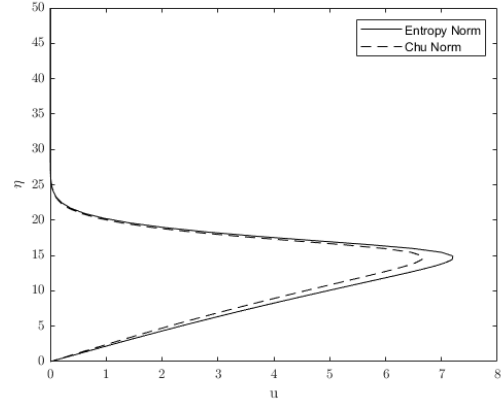


((d)) Optimal temperature output mode

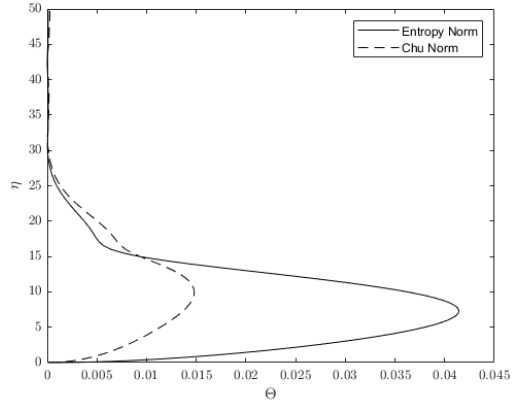
Figure 5.8: Optimal input and output disturbance in a Mach 1, adiabatic wall condition boundary layer with $\alpha = 0$ and $\beta = 0.1$ and a Reynolds number of 300



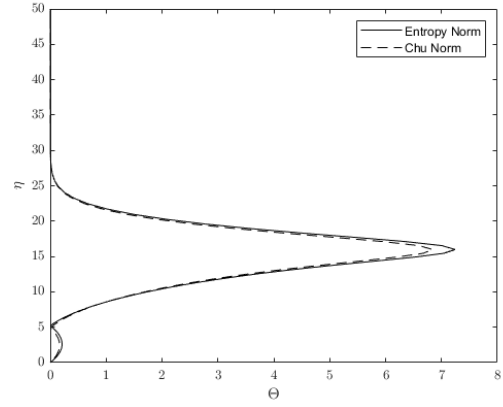
((a)) Optimal velocity input mode



((b)) Optimal velocity output mode

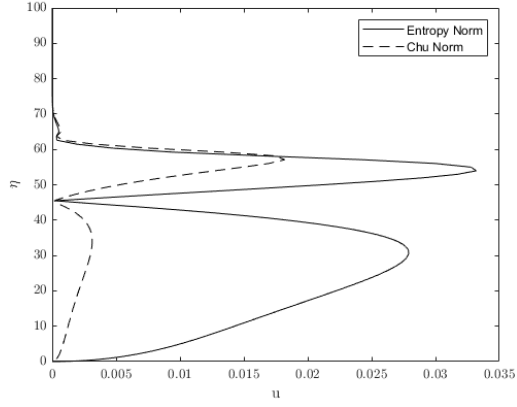


((c)) Optimal temperature input mode

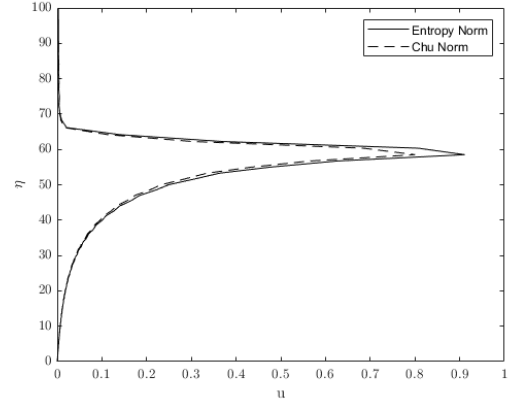


((d)) Optimal temperature output mode

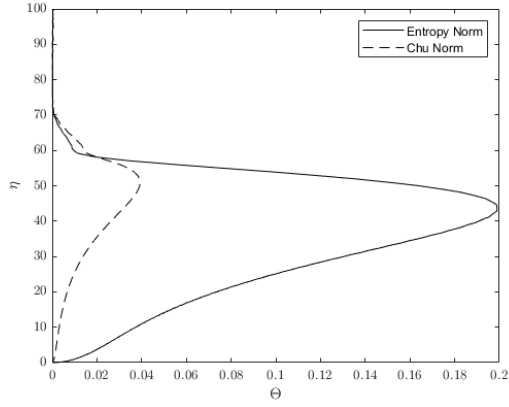
Figure 5.9: Optimal input and output disturbance in a Mach 5, adiabatic wall condition boundary layer with $\alpha = 0$ and $\beta = 0.1$ and a Reynolds number of 300



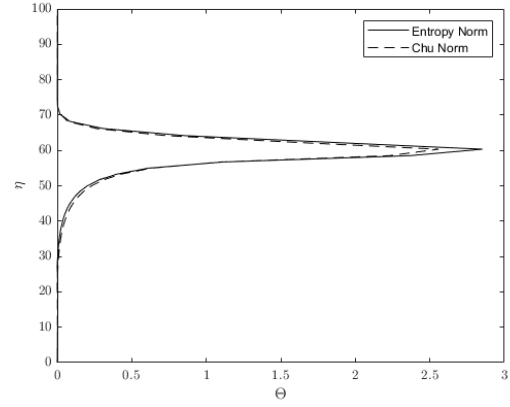
((a)) Optimal velocity input mode



((b)) Optimal velocity output mode



((c)) Optimal temperature input mode



((d)) Optimal temperature output mode

Figure 5.10: Optimal input and output disturbance in a Mach 10, adiabatic wall condition boundary layer with $\alpha = 0$ and $\beta = 0.1$ and a Reynolds number of 300

the velocity perturbation in the optimum output is generally constant across the Mach number sweep, but the temperature perturbation experiences a significant increase in magnitude as Mach number increases. The increasing importance of temperature appears to closely align with the divergence of the amplification profiles predicted by each norm. It is suggested by the mathematical relationship between the norms that temperature is the driving factor in this divergence, and that the entropy norm is more sensitive to temperature disturbances than the energy norm. It should also be noted that, in the examination of the amplification profiles, the entropy norm was found to predict higher gain in cases where the overall temperature magnitude inside the boundary layer, especially near the wall, is higher. Overall these findings demonstrate consistency with the mathematical exploration of the norm behavior and general understanding of thermodynamic contributions to viscous compressible flows.

Summary and Discussion

In general, the results obtained from this linear stability analysis demonstrate the properties expected from the entropy normalization relative to the Chu normalization as explored mathematically. The results found through the study of non-modal growth provide a good means to establish expectations of what each normalization will predict in POD applications. The jet in crossflow is better suited to examining qualitatively the modes output from POD analysis to compare the features highlighted by each normalization and the modal energy spectrum of each decomposition implementation.

While it has been stated already that the two norms predict the same features but different relative magnitudes, the entropy norm has advantages in light of the instability mechanisms typical of high-speed flows. Qin and Wu [141] describe three types of disturbances which may instigate instability in compressible boundary layers. These are acoustic disturbances, which includes a velocity, density, and temperature component (usually thought of as pressure), vortical disturbances, which contain only a velocity component, and entropic perturbations, which contain only a temperature

perturbation. When any of these strikes a shockwave, it causes the shockwave to oscillate, meaning the boundary layer behind the shock is subject to all three types of disturbances. Moreover, the Mack-mode instabilities to which transition is commonly attributed in hypersonic flows are documented to be excited by wall cooling and mitigated by the existence of a large entropy layer. These two trends are related to the temperature gradient near the wall. As demonstrated here, the entropy norm is much more sensitive to temperature gradients, introduced either by modulating the wall temperature or by increasing Mach number. This is particularly true of the Mach 10 mode shape, where the Chu norm predicts velocity perturbations as the dominant disturbance features, but literature examining the morphology of instabilities suggests that thermodynamic disturbance should also play a role. By contrast, the entropy norm predicts thermodynamic disturbances increasing in importance as the temperature gradients inside the boundary layer grow, which is known to destabilize the boundary layer by better amplifying acoustic disturbances trapped near the wall.

Chapter 6

Application to Modal Decompositions

Data Source Statement

The analysis of a homogenous jet-in-crossflow was originally conducted for a submission to the Journal of Theoretical and Computational Fluid Dynamics which is currently under review for publication, and has been adapted for inclusion here. Analysis of the cone-slice-ramp was conducted for submissions to AIAA Aviation 2019, SciTech 2020, and SciTech 2021.

6.1 Test Cases

6.1.1 Single-Species Jet in Crossflow

Simulation of the jet-in-crossflow was performed with OVERFLOW 2.3 [142]. OVERFLOW is a structured overset flow solver which offers the advantage of fitting high-order stencils over complex geometries. OVERFLOW is capable of performing RANS and implicit large-eddy simulation (ILES) analysis. ILES simulations resolve larger turbulent eddies and allow numerical dissipation to act as a subgrid turbulence model to approximate scales smaller than the grid resolution. It is an intermediate

between RANS, which does not capture transient phenomena, and direct numerical simulation (DNS), which would be cost-prohibitive for this analysis. Grids used in this research were generated in Pointwise and Chimera Grid Tools [143]. Grid spacings for all cases were determined using industry best practices for overset grids [144], and data about boundary layer thickness can be used to inform the spacings of ILES grids. For ILES, non-dimensional wall spacings are a $\Delta x^+ 100$, a near-wall $\Delta y^+ = 0.1$, and a $\Delta z^+ of 30$, where Δy^+ is normal to the wall, are used. Overall the final mesh size was approximately 47 million grid points in a single block. In order to ensure stability of the solution, ILES cases run in OVERFLOW are primed using a multi-step process. All cases were first run in a steady-state configuration to allow a pressure and velocity field which is approximately the mean of the unsteady solution to set up. From there, the simulations were switched to time-accurate and allowed to flush the influence of the steady-state solution from the domain before data collection began.

All cases used an HLLE++ upwinded scheme [145] with a 5th-order WENO reconstruction. For places where heat flux is desired, it is calculated using Sutherland’s law [146]. All cases used an SSOR algorithm with five Newton sub-iterations and a non-dimensional time step of $\Delta t = 0.001$. In order to reduce grid size requirements associated with developing a boundary layer profile, each case used a preliminary run which matched the numerical and flow conditions of the final run, but did not include the jet. These preliminary cases were converged to generate developed flat-plate boundary layer profiles which were extracted and used as a custom boundary condition on the inflow plane to the computational domain. Each case was run with a Reynolds number of 1000 based on the jet radius and a free-stream Mach number of 4. For this application, a homogeneous jet was chosen to eliminate unnecessary complexity. In order to eliminate potential errors associated with overset grid boundaries, the jet grid is embedded into the flat plate grid as shown in Fig. 6.1.

Points inside of the circle are subject to an inflow boundary condition while points everywhere else are subject to an adiabatic wall boundary condition. Cases were run

with the default free-stream temperature of 396 R. The jet was "cold" and under-expanded. Its total temperature was set to be $\frac{1}{3}$ of the free-stream and a total pressure 4 times higher than the free-stream.

6.1.2 Two-Species Jet-in-Crossflow

For the two-species jet-in crossflow, the grids were re-generated to accommodate a larger SWBLI recirculation region. The upstream inflow plane was moved upstream to accommodate the SWBLI, and the domain was stretched so that the spacing in the plume region was as uniform as possible. This grid was constructed using a similar set of non-dimensional wall spacings: a $\Delta x^+ = 100$, a near-wall $\Delta y^+ = 0.1$, and a $\Delta z^+ of 30$. The inflow boundary layer profile was generated using same method employed for transient growth analysis. 2-D profile generated this way was projected onto the inflow plane using custom FORTRAN routines. Overflow is capable of solving for flows with multiple species, but there is no default boundary condition which allows for inflow of a different composition than the free-stream. The custom boundary condition was used to circumvent this limitation, as the custom inflow condition could be used to set the gas properties and composition as well as the density, momentum, and energy profiles. For this case, air was used as the free-stream flow and the jet is composed of methane.

In overflow the species equation is loosely coupled to the solution of the conservation equations, but the values of the species equations are updated at each newton subiteration, so the time-accurate ILES conducted here couples the two more tightly than in the preconditioning steps. In order to increase the coupling of the species and kinematic equations for this case, it was run with ten newton subiterations as recommended by the developers of OVERFLOW [142].

6.2 Results

6.2.1 Single-Species Jet in Crossflow

The jet-in-crossflow was chosen for this analysis because it provides a favorable combination of temperature gradients, instabilities, and reasonable computational cost for evaluating norm behavior with POD. Before analyzing the modal behaviors found in the jet in crossflow, its basic dynamics should be explored to establish expectations for the predominant unsteady regions. Fig. 6.2 shows the mean profile for the Mach 4, adiabatic wall case of the jet in crossflow alongside a representative transient snapshot. While the jet-in-crossflow is a very well-characterized test case, it is still worthwhile to examine the base flow to highlight the regions which exhibit significant dynamic behaviors and temperature gradients. The SWBLI region at the base of the jet exhibits significant dynamics, and the interface between the jet fluid and the free-stream flow behind the bow shock is subject to vortex instabilities which induce sharp temperature gradients and rotation. There are also strong temperature gradients in the SWBLI recirculation region at the base of the jet plume. This region demonstrates unsteadiness as well, making it another strong candidate for comparison. The shockwave visible in the upper right hand corner of the figure emanates from the simulated leading edge of the flat plate case used to generate the incoming boundary layer profile. Because the boundary layer was extracted so as to generate an interaction when the boundary layer is approximately the same thickness as the jet diameter, the shock from the inception region of the boundary layer is captured in the extracted slice and propagates into the interaction simulation. The domain shown is that extracted for POD, which was selected to contain the dynamics of the jet but not the large cells in the far-field. The SWBLI extends further upstream than this sub-domain, but it terminates prior to the inlet of the domain for the time steps included in POD calculations, though the SWBLI was found to expand as the simulation continued. For this reason, the grids for the multispecies jet were

extended farther upstream. This case required more refinement in the plume region to achieve high-quality results because of the loose coupling between the species and flow equations as implemented in OVERFLOW. Without this refinement, the species mass fraction distribution is often observed to be aligned along the grid.

6.2.2 Multispecies Jet-In-Crossflow

Compared to the single species case, the multispecies jet-in-crossflow exhibits some phenomenological differences owing to the difference in gas properties of the jet flow. Methane is, for the same conditions, much less dense than air and therefore the methane jet does not carry the same momentum into the free-stream as the single species jet does. The, combined with the entrainment and expansion of methane from the jet into the SWBLI upstream of the inflow leads to a much shorter plume and larger SWBLI region. The SWBLI region extends to the top of the jet plume regardless of jet pressure ratio for all iterations of the jet attempted, and most of the dynamics of the jet are found in the upper plume and wake. The SWBLI region is dynamic as well, though as in the incompressible case the temperature gradients are smaller here. Of critical interest is the distribution of methane in the SWBLI and jet plume. Fig 6.3 shows a representative snapshot of the multispecies jet in crossflow along with the time-averaged solution for the domain studied here. Immediately of interest is the observation of methane recirculating upstream inside the SWBLI and diffusing upstream below the sonic line of the boundary layer. It is observed that this diffusion does not reach all the way to the inflow plane, whose species composition and properties are dictated by the boundary condition. In order to accommodate the large SWBLI region, the inflow plane for this case was made to be significantly longer than the single-species case. Of interest in this case is the unsteadiness in the jet-freestream interface, including the diffusion that happens across this interface. The SWBLI is of greater interest in this case as a site of mixing and because the SWBLI is large enough that unsteadiness from the SWBLI spills over the top of the

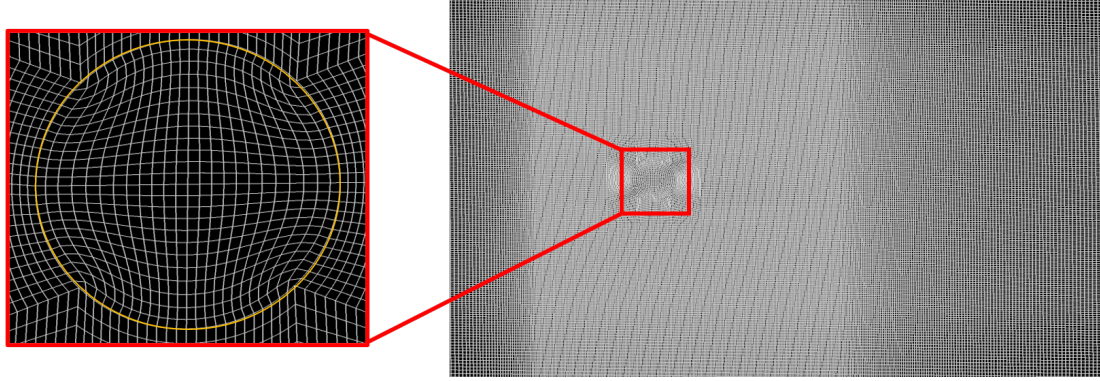


Figure 6.1: Topology of jet-in-crossflow test case showing circular jet embedded in the Cartesian grid. This figure has been trimmed for clarity

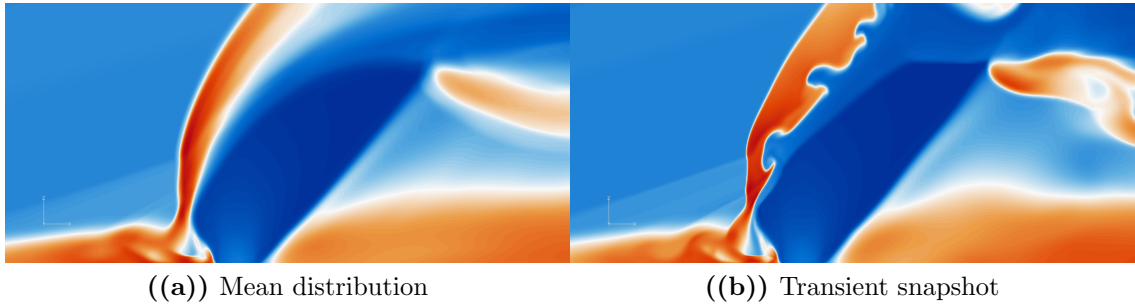


Figure 6.2: Mean and transient temperature profile of a cold, high-pressure jet in relatively warm, Mach 4 cross-flow with an adiabatic wall

jet plume. The importance of this region is seen in Fig. 6.4, which shows the hot gas from the SWBLI interacting with the stagnation point at the intersection of the jet, the SWBLI, and the free-stream. The wake region near the jet is also of interest, again as a location of dynamic gas composition. As in the single-species case, the region at the interface between the jet and the freestream flow houses roller-like instabilities which are a prominent source of dynamic behavior.

6.3 Modal Decomposition

For this study, snapshot POD was implemented in FORTRAN using Open MPI for parallelization. In order to mitigate the influence of flow quantities in the far-field where the grid is coarse, those regions have been excluded from POD calculations using OVERFLOW's built-in subdomain extraction capabilities. For each case three POD implementations were used, one with the Chu norm, one with the dense entropy norm calculated from the entropy variables, and one with the diagonal entropy norm calculated by mapping from the primitive variables to entropy. These implementations are compared to one another to examine the phenomenological differences in the features captured by each mode of each decomposition, and the modal energy distribution in each of them.

6.3.1 POD Analysis of Jet-in-Crossflow

The first relevant result of POD analysis is the identical eigenspectrum and mode shape of density modes calculated with the two different formulations of the entropy norm. As shown in Fig. 6.5, the modal energy distribution in all of these compositions demonstrates a nearly identical distribution of modal dynamic contents. For the case of the two entropy norms, these distributions are in fact identical. These two normalizations do not have identical eigenvalues, but the ratio of each eigenvalue relative to the sum of all of the eigenvalues is the same, which is a result of the

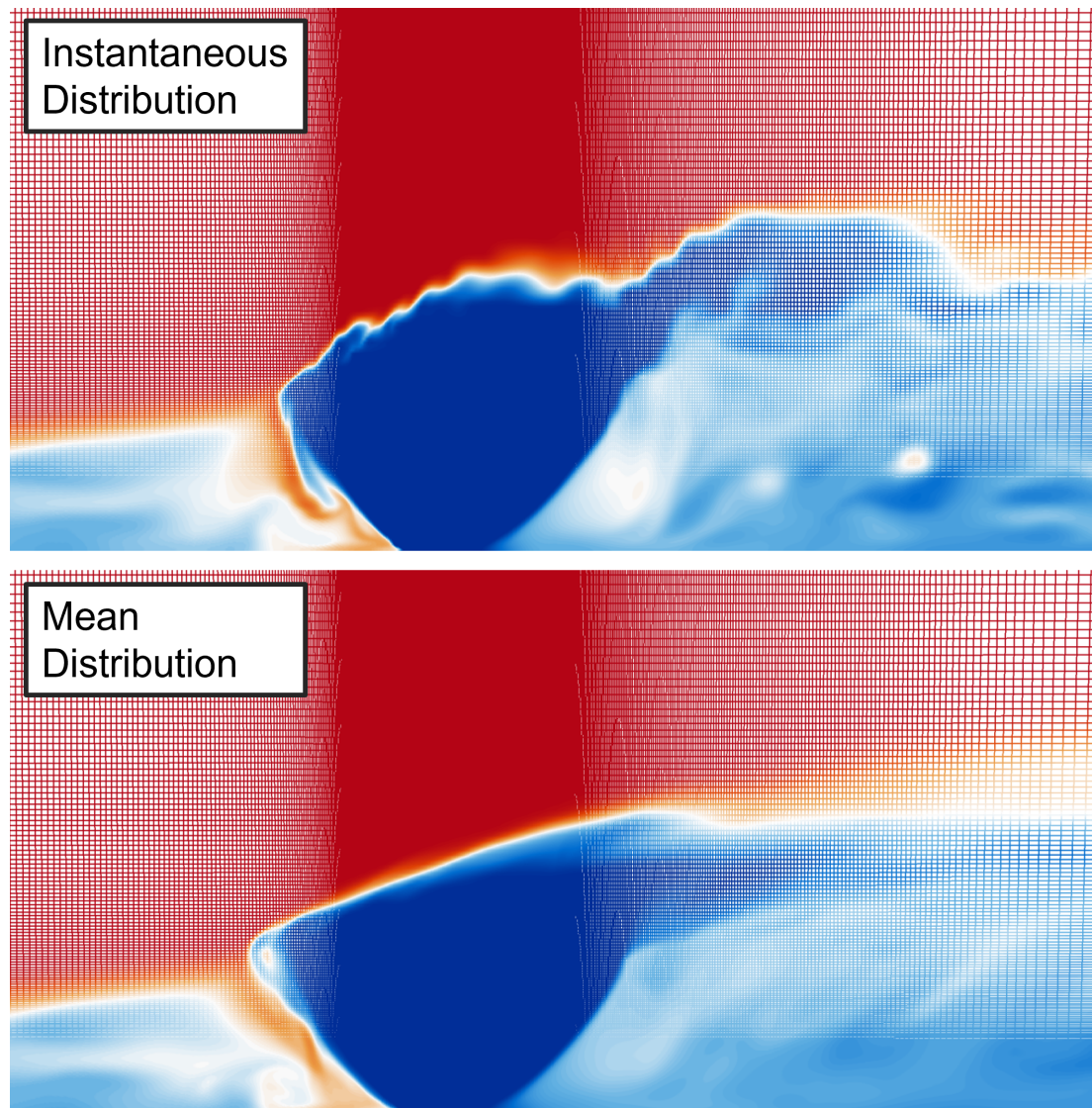


Figure 6.3: Species distribution in the multispecies jet-in-crossflow. Red corresponds to air and blue corresponds to methane

different normalizations contracting against different quantities. For both cases the first variable in the relevant set is density, hence the focus placed on modes of densities in comparing normalizations to one another. For a POD analysis this modal dynamic content distribution is somewhat unfavorable, but the distribution is a function of the case itself as well as the normalization. While it does not appear that the entropy norm has any significant advantage in series convergence over the Chu norm, it also does not appear as if its behavior is significantly less favorable.

The coincidence of the two entropy implementations confirms that these are in fact two statements of the same norm, and the diagonal, primitive-variable entropy norm is omitted from mode spatial distribution plots because it adds no new information. Based on the analysis of self-similar boundary layers, it is expected that POD modes calculated with each normalization will demonstrate close agreement in global behavior, but may predict differences in local features in the presence of strong temperature gradients. For the jet-in-crossflow these regions of possible disagreement would be the interface between the shock wave and the jet and the re-circulation region on the front of the jet at the wall. Comparing first modes of density calculated with the entropy and Chu norms shown in Fig. 6.6 shows this expected behavior. The Chu and entropy norm agree very closely on most features. Close inspection shows that at the region near the mach disc on the top of the jet the Chu norm appears to smear some features which are shown in more detail with the entropy norm. The oscillatory content of the heterogeneous vortex appears to remain more coherent with the entropy norm as this feature advects upwards with the jet. Additionally, the jet itself is seen to contain more content in the mode calculated with the entropy norm. The SWBLI away from the wall appears to be more pronounced with the Chu-calculated mode.

The second mode shows that the entropy mode still places more emphasis on the dynamic behavior of the jet itself. In some regions of the heterogeneous vortex structures the Chu norm shows features very similar to those the entropy norm predicted in mode 1. The entropy norm also shows dynamic content from the

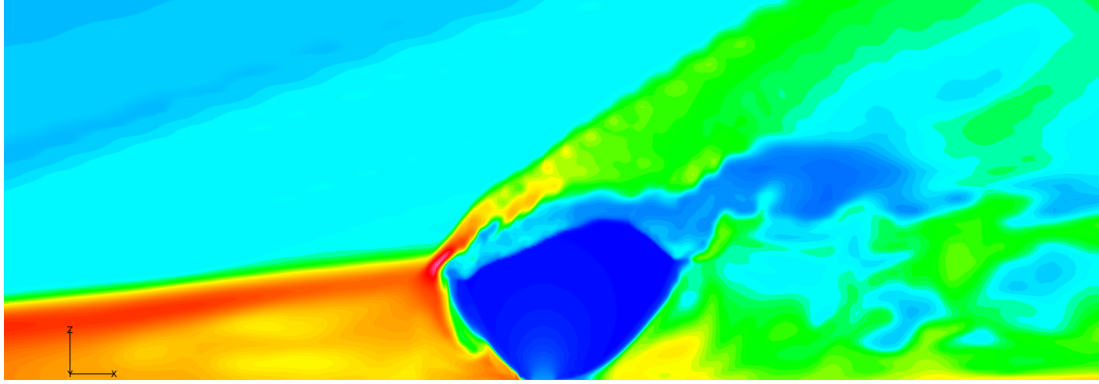


Figure 6.4: Instantaneous temperature contour of the multispecies jet-in-crossflow. The SWBLI is seen to be a greater source of thermal activity in this case than was observed in the single-species case.

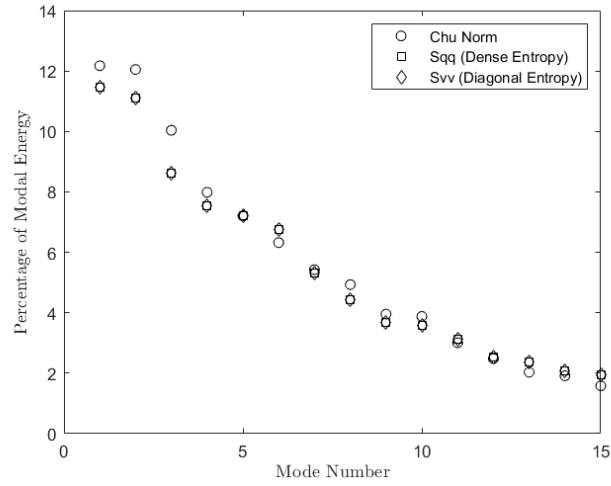


Figure 6.5: Distribution of dynamic behavior calculated through eigenvalue dropoffs for the Chu norm and both implementations of the entropy normalization. Dynamic content distributions for the conservative entropy norm and the primitive entropy norm are identical

SWBLI radiating farther upward than is seen in the Chu-calculated mode. The Chu norm placing greater relative focus on the SWBLI is consistent with its expected greater interest in the kinematic portion of flow dynamics. The interaction between the jet and the free stream creates a much larger temperature gradient than the SWBLI, so in the context of the jet-in-crossflow the SWBLI's contribution to the flow is largely kinematic instead of thermodynamic. Finally, in the second mode the entropy norm appears to identify perturbations in density away from the dominant flow features which are not present in the Chu norm. This phenomenon is seen in the SWBLI and behind the Mach disc below the advecting vortex content. As seen in the transient growth calculations, temperature perturbations can exist outside of dominant kinematic features, and it is possible that small temperature perturbations (felt as density perturbations) are present here and are detected by the temperature-sensitive entropy norm. To investigate this more thoroughly, it would be necessary to examine a test case which is known to produce similar fluctuations, such as a thermal instability.

The modes calculated with the Chu norm are subtracted from the corresponding modes calculated with the entropy norm, which helps to highlight regions of disagreement. This comparison is shown in Fig. 6.7. In this figure, it is seen that there is mild disagreement over large regions of the jet-shock interaction region, but the largest differences in modes one and two are found at the edges of the jet plume and in the region where the SWBLI impinges on the expanding cold jet. These are regions of sharp temperature gradients, and this localized disagreement is in keeping with the observations made in the analysis of transient growth of compressible boundary layers and from the examination of the role of entropy in Navier-Stokes systems. For the case of the Mach 4 jet-in-crossflow, the low total temperature of temperature of the jet introduces temperature gradients into the flow which would not be expected for external flows with adiabatic boundary conditions at similar Mach numbers. In this figure the SWBLI upstream of the jet is a region where the temperature gradients are generated entirely by the compressibility of the flow, and it is clear that this is

insufficient to force significant disagreement. This too is consistent with transient growth analysis which showed some deviation in the mode shapes at Mach numbers around 5. This deviation grew more pronounced as Mach numbers increased further. Temperature gradients in the jet-shock interaction region are comparable to those observed for Mach numbers above 5 in the transient growth analysis, this region should be expected to display substantial differences in the modes between the norms.

Overall, the jet-in-crossflow analyzed here demonstrates that the behaviors found in transient growth analysis hold in applications to three-dimension compressible flow POD. The entropy norm agrees very closely with the Chu norm for most regions of the flow, but disagreement appears in regions with high local temperature gradients. Theory and transient growth analysis results predict that for cases where compressibility is even stronger, this disagreement will be exacerbated, and the agreement between theory, transient growth analysis, and applied POD for all conditions examined leave little reason to doubt these predictions.

6.3.2 POD Analysis of Multispecies Jet in Crossflow

Of interest in examining the methane jet in air crossflow is the impact of mixing on the resulting POD modes. In developing the norm, it was remarked that an entropy of mixing was unnecessary because the calculation was not based on a total pressure. While the simulation in question here considers each gas to be of constant properties, each gas has a different γ and so the thermodynamic properties of the mixture vary between those of air and those of methane. Because of the way species conservation is enforced in OVERFLOW, the simulation calculates the gas properties separately using species continuity and then calculates the rest of the flow variables using the resulting mixture properties. This means that the solution stores total density and individual species densities separately. A POD implementation has been developed for flows with multiple species. The algorithm is otherwise identical to the baseline entropy-contracted POD routine using the diagonalized norm. This POD

tool has been used to examine the methane jet in air crossflow. Examples of the decomposition results using the multispecies POD routine are shown in Fig. 6.8. An unsurprising result is that the modes for each gas have no content where the mass fraction their corresponding gas is zero. This is an expected validation, but also suggests potential utility for this type of analysis. For some applications, such as in combustion problems, it may be desirable to examine the unsteady behavior of specific constituents. It is also observed that the structures in the jet-shock interface are less coherent in the total density mode than in either of the single species modes. It is suspected that the mixing of fluids with different densities in that region is interpreted as noise in the mixture density calculation, but the individual modes do not capture this interference.

Examining temperature modes in 6.9, which are calculated the same way in both decompositions, finds the two decompositions predict identical features. These figures are shown side-by-side rather than one subtracted from the other to avoid the small error in the density calculation from the loose species coupling causing error causing the difference to be misleading.

The eigenvalue dropoff, corresponding to the total perturbation entropy described by each mode, is shown in Fig 6.10. This figure shows close agreement between the two analyses. In calculation of the computation using mixture properties, the individual species densities must still be referenced in the construction of S_{vv} because the specific gas constant is no longer a uniform value. Overall, the multispecies implementation exhibits favorable properties in eigenvalue decay for a POD analysis.

6.3.3 Summary and Discussion

The jet in crossflow provides an opportunity to examine the entropy norm for a case with significant temperature gradients whose behavior is well characterized in the literature. Consistent with the behaviors observed in transient growth analysis, the

entropy normalization is observed to highlight regions with significant temperature gradients.

From these results alone, it is very difficult to make a judgment of which normalization is better for general use beyond those which rely on the mathematical arguments outlined in the derivation of the entropy norm. Nevertheless, the entropy normalization does have one advantage in reduced order modeling. Because the eigenvalues corresponding to each mode represent the fraction of dynamic content represented by it. Because the entropy normalization defines this dynamic content to be entropy, a reduced order model built using the entropy normalization will, by construction, converge as quickly as possible to a solution which satisfies the second law (an entropy solution).

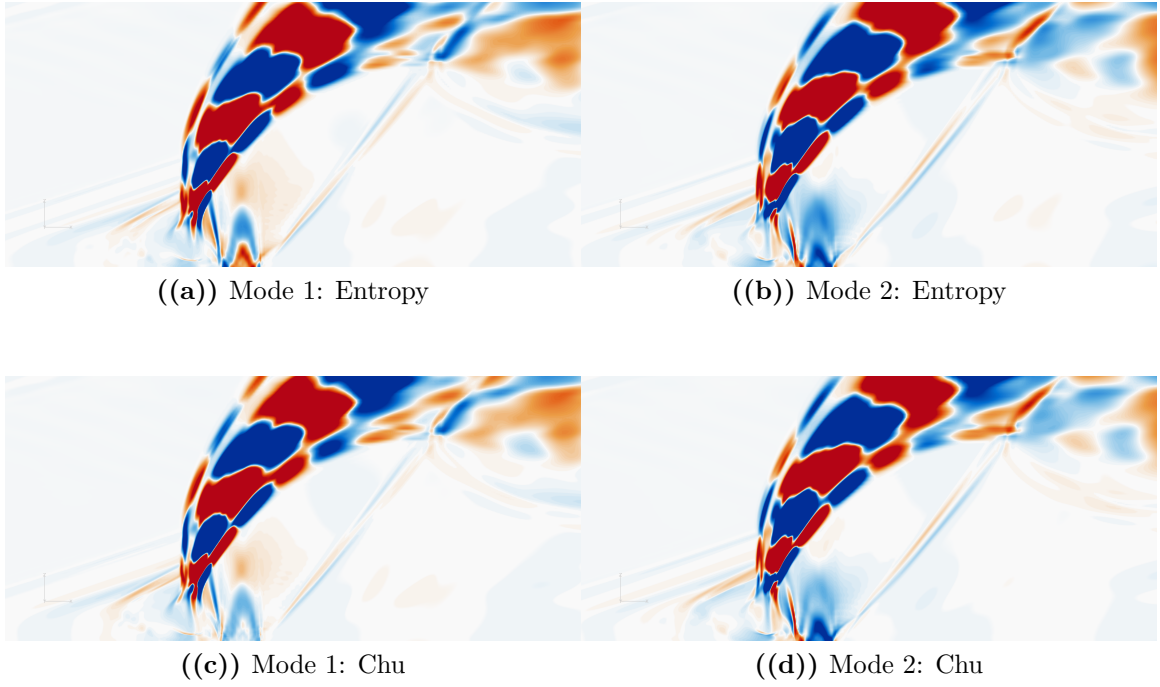
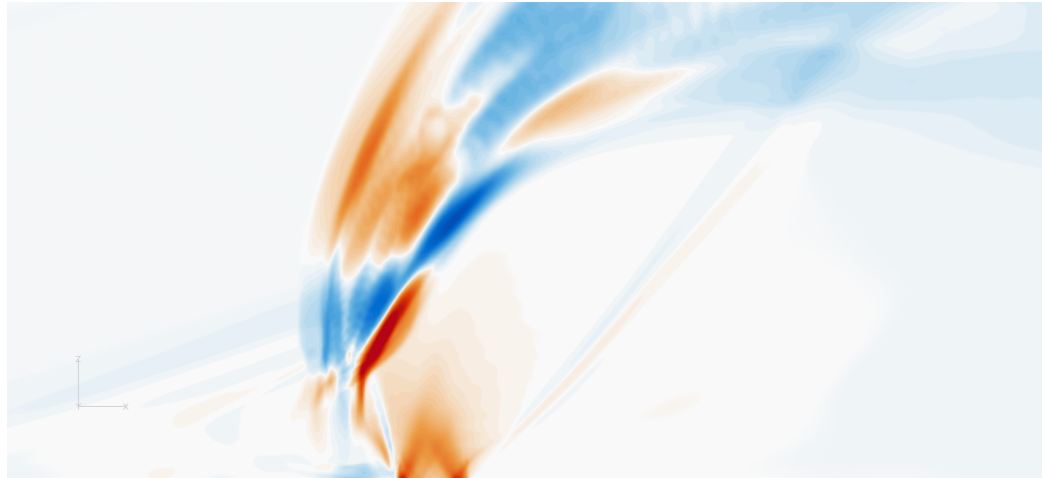
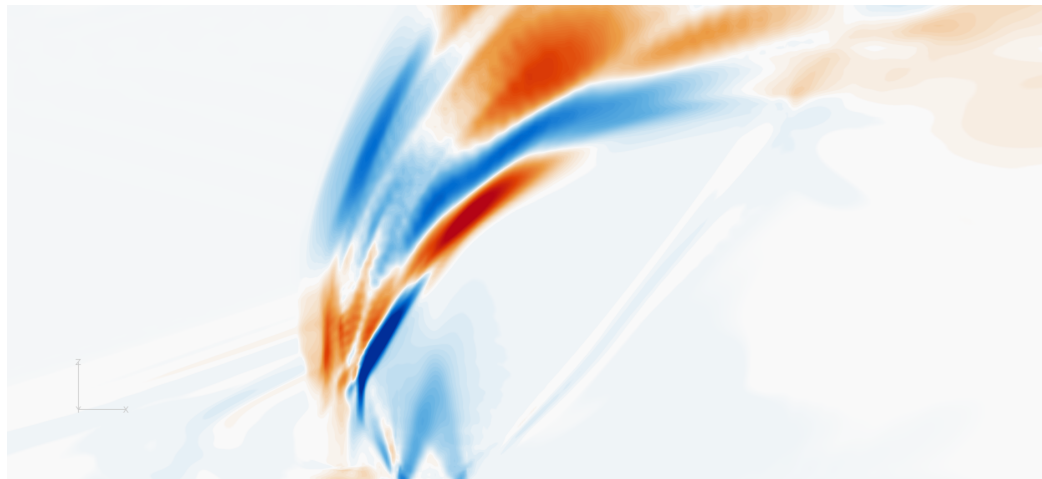


Figure 6.6: First two modes of density for a cool jet in Mach 4 hot crossflow with an adiabatic wall. Decompositions are calculated with the same 100 snapshots



((a)) Mode 1 difference



((b)) Mode 2 difference

Figure 6.7: Variation between Chu-calculated modes and Entropy-calculated modes for the jet-in-crossflow

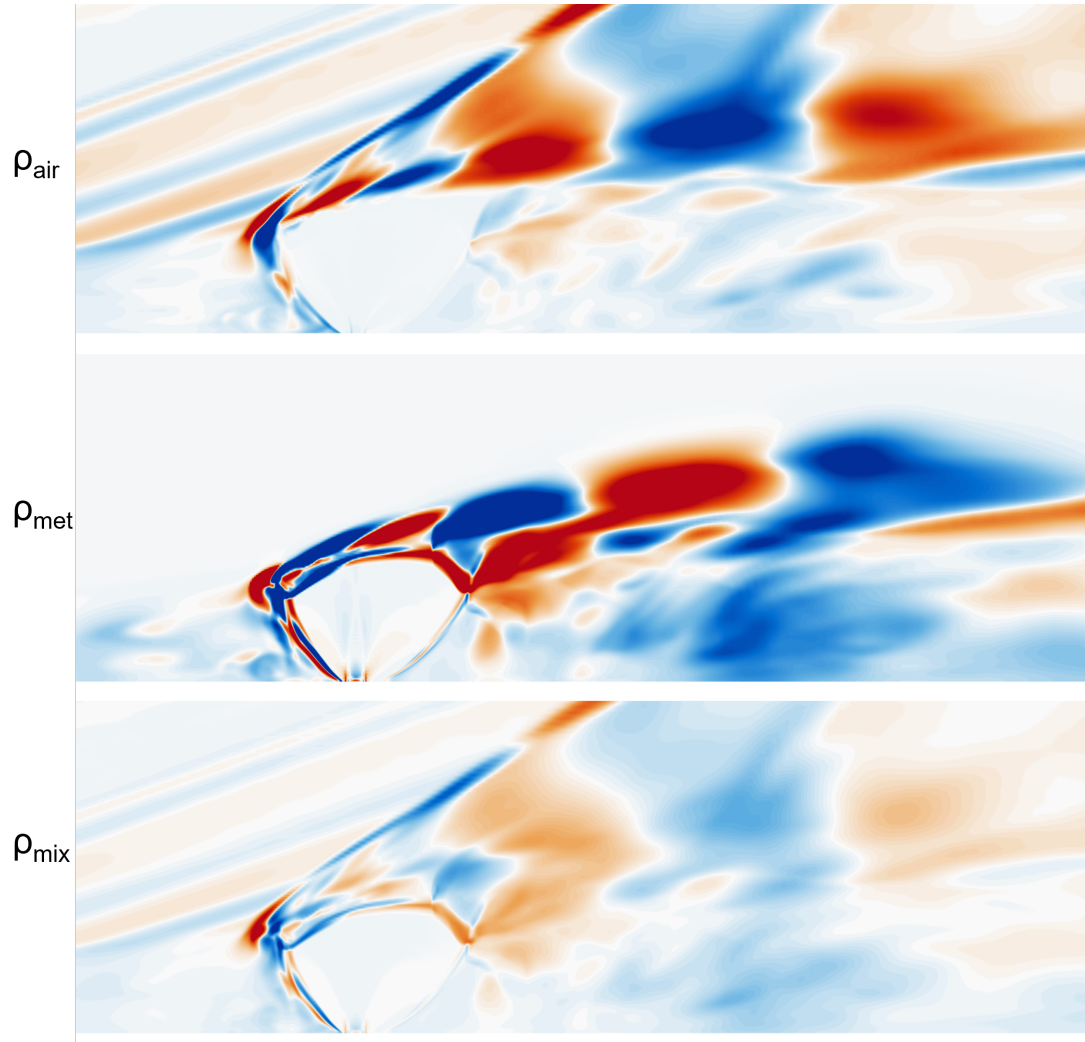


Figure 6.8: First mode of density for each species for a cold methane jet into relatively hot, Mach 4 air crossflow

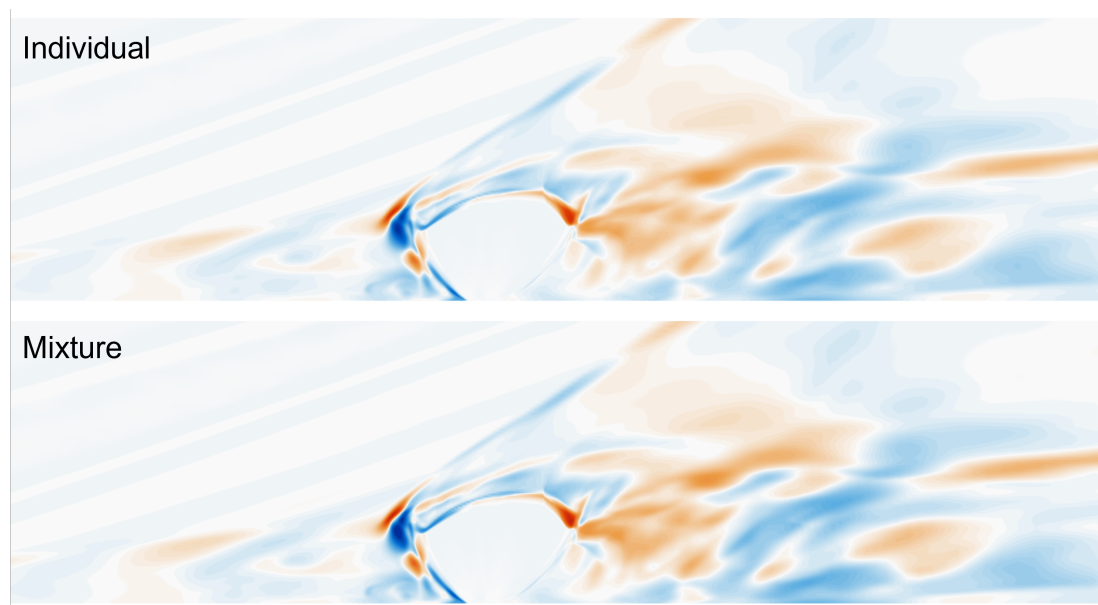


Figure 6.9: First mode of temperature calculated with individual species properties and with mean flow properties

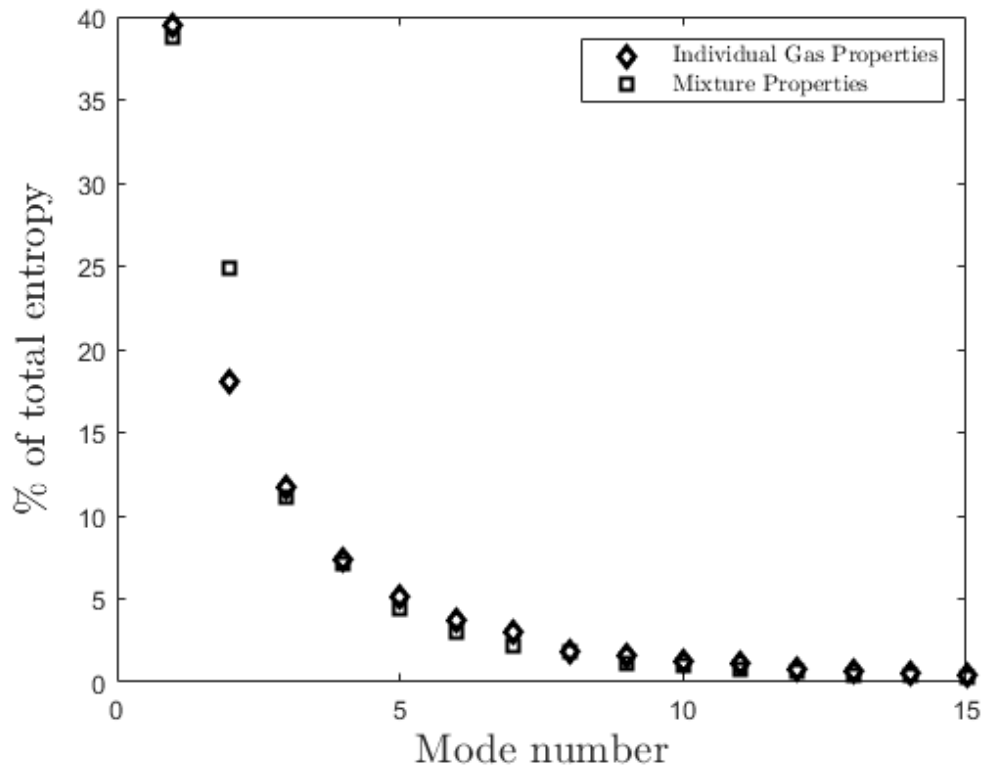


Figure 6.10: Eigenvalue drop off in the multispecies POD calculation compared to the equivalent calculation using total density and mixture properties.

Chapter 7

Entropy of Isotropic Turbulence

7.1 Computational Approach

The numerical solver employed in the analysis of isotropic turbulence is an emerging finite volume tool from the volAIR research group at the University of Tennessee, Knoxville. The main branch of the code is a high-order, LES solver called the Wall-Resolved Body-Fitted Large Eddy Simulation (WRBLES) solver. The code is written in FORTRAN and parallelized using intel MPI. The finite difference solver employs the upwinded inviscid flux eigenvectors of Pulliam et al. [147] with a 5th order WENO reconstruction. The inviscid fluxes were calculated using Roe averaging at the cell interfaces [148].

A branch of the code has been developed for this work to implement vibrational energy storage and thermal nonequilibrium to the solver. This version of the code is called Two-Temperature Wall-Resolved Body Fitted Large Eddy Simulation (TWRBLES) solver, and solves the Navier-Stokes equations with a single additional energy equation which tracks vibrational energy. Vibrational relaxation is grouped with the viscous processes and the inviscid terms are treated with the other conservative variables and fluxes. TWRBLES uses the the inviscid flux formulation presented by Gnoffo [27], and the vibrational nonequilibrium terms implemented

as described by Park [124], which uses the Landau-Teller model for vibrational relaxation. Because the goal of the analysis is to examine the impact of the various gas and flow parameters on the entropy production, vibrational relaxation time is a prescribed constant value rather than a function of the local thermodynamic state, as suggested by Park. Vibrational energy is calculated from vibrational temperature using the analytic relation derived from statistical mechanics by treating molecules as harmonic oscillators as described by Vincenti and Kruger [149]. The TWRBLES code operates using nondimensional variables as follows,

$$\begin{aligned}
x^* &= \frac{x}{L} \\
V^* &= \frac{V}{a_\infty} \\
t^* &= \frac{ta_\infty}{L} \\
R^* &= 1 \\
T^* &= \frac{T}{\gamma_\infty T_\infty} \\
T_v^* &= \frac{T_v}{\gamma_\infty T_\infty} \\
\theta^* &= \frac{\theta}{\gamma_\infty T_\infty} \\
\rho^* &= \frac{\rho}{\rho_\infty} \\
p^* &= \frac{p}{\rho_\infty a_\infty^2} = \frac{p}{\gamma_\infty p_\infty} \\
C_{v,tr}^* &= \frac{C_{v,tr}}{R} \\
C_{v,v}^* &= \frac{C_{v,v}}{R} \\
e_v^* &= \frac{e_v}{a_\infty^2} \\
e_{tr}^* &= \frac{e_{tr}}{a_\infty^2}
\end{aligned} \tag{7.1}$$

where γ is the ratio of translational-rotational specific heats, and so is still 1.4 for diatomic species even in the case of a calorically imperfect, nonequilibrium gas. A practical implication of these nondimensionalizations is that the relationship between T_v and e_v is dependent on the reference temperature since the characteristic vibrational temperature is always a dimensional quantity specific to the working fluid. Introducing vibrational nonequilibrium significantly reduces the acceptable time step for the simulation. Because the vibrational time scale is small, coarse temporal discretization leads to fatal overshoot of the vibrational relaxation at a given time step.

Inviscid flux terms are treated using the eigenvalues provide by Gnoffo [27], adapted to consider only vibrational temperature and a single species. The resultant upwinded flux Jacobian, $\frac{\partial f}{\partial q} = A = L\Delta R$, is

$$\mathbf{R} = \begin{bmatrix} a^2 - \bar{\gamma} & \beta u & \beta v & \beta w & -\beta & -\phi \\ -V & l_x & l_y & l_z & 0 & 0 \\ -W & m_x & m_y & m_z & 0 & 0 \\ \bar{\gamma} - Ua & an_x - \beta u & an_y - \beta v & an_z - \beta w & \beta & \phi \\ \bar{\gamma} + Ua & -an_x - \beta u & -an_y - \beta v & -an_z - \beta w & \beta & \phi \\ -e_V \bar{\gamma} & \beta u e_V & \beta v e_V & \beta w e_V & -\beta e_V & a^2 - \phi e_V \end{bmatrix} \quad (7.2)$$

$$\mathbf{L} = \begin{bmatrix} \frac{1}{a^2} & 0 & 0 & \frac{1}{2a^2} & \frac{1}{2a^2} & 0 \\ \frac{u}{a^2} & l_x & m_x & \frac{u+an_x}{2a^2} & \frac{u-an_x}{2a^2} & 0 \\ \frac{v}{a^2} & l_y & m_y & \frac{v+an_y}{2a^2} & \frac{v-an_y}{2a^2} & 0 \\ \frac{w}{a^2} & l_z & m_z & \frac{w+an_z}{2a^2} & \frac{w-an_z}{2a^2} & 0 \\ \frac{\beta(u^2+v^2+w^2)-\bar{\gamma}}{\beta a^2} & V & W & \frac{(H+aU)}{2a^2} & \frac{(H-aU)}{2a^2} & -\frac{\phi}{\beta a^2} \\ 0 & 0 & 0 & \frac{e_V}{2a^2} & \frac{e_V}{2a^2} & \frac{1}{a^2} \end{bmatrix} \quad (7.3)$$

and

$$\Delta = \text{Diag}[U, U, U, U + a, U - a, U] \quad (7.4)$$

where the quantities β , ϕ , and $\bar{\gamma}$ are the thermodynamic closures required to appropriately incorporate the vibrational temperature. These are taken as-is from Gnoffo so as to facilitate future upgrades of the code's nonequilibrium capability, even though some are redundant in the it current form. The quantities are defined as

$$\beta = \frac{\partial p}{\partial \rho E} = \frac{R}{\rho C_{v,tr}} \quad (7.5)$$

$$\phi = \frac{\partial p}{\partial \rho e_V} = -\beta \quad (7.6)$$

which includes an additional electronic pressure term if those effects are considered, and

$$\bar{\gamma} = \frac{\partial p}{\partial \rho} = RT + \beta \frac{u^2 + v^2 + w^2}{2} - \beta e - \phi e_V \quad (7.7)$$

The vectors l , m , and n are mutually orthogonal unit vectors, where l is the unit vector normal to the cell face and the other two vectors are randomly-generated and then orthonormalized using the Gram-Schmidt process. Simulations were run on the Secure Enclave portion of UTK's ISAAC facility. For the sake of consistency, all analyses were run using the TWRBLES branch of the WRBLES framework. For cases where vibrational nonequilibrium is not a quantity of interest, the addition of the vibrational energy terms does not harm the solution beyond the imposed time step requirement.

One goal of this analysis was to examine the relative importance of the entropy generation of the vibrational relaxation process compared to the other entropy sources in the flow. This term is influenced by the characteristic vibrational temperature and the vibrational relaxation time of the gas. For this study, the working fluid is taken to be a generic diatomic gas because the nondimensionalization removes all dependence on R for a constant-composition simulation, and the vibrational relaxation parameters

are varied to examine the relative influence of each on the overall entropy generation. In order to characterize the initial conditions in these terms, two new non-dimensional parameters are introduced,

$$\Psi = \frac{\theta_v}{T_\infty} \quad (7.8)$$

$$\Theta = \frac{\tau_{inv}}{\tau_{v-t}} = \frac{2\pi}{u_{rms}\tau_{v-t}} \quad (7.9)$$

where Ψ will heretofore be referred to as the vibrational excitability, and Θ is the vibrational Damköhler number as suggested by Fujii and Hornung [150] and studied by Neville [112]. The definition for vibrational Damköhler number used here is slightly different than that used by Neville because the study undertaken here examines a wider variety of initial conditions than Neville's analysis and the chosen definition is consistent across all of these. The vibrational excitability describes the potential of the gas for vibrational excitation without respect to the relaxation process, and the vibrational Damköhler number describes the relative time scale of the vibrational relaxation process compared to the turbulent scales. As the vibrational excitability approaches 0, the gas approaches saturation of the vibrational mode (and therefore constant $C_{v,v}$). At large values, there is not enough energy in the flow to excite the vibrational mode to detectable levels, and the flow is calorically perfect. At very small values of the vibrational Damköhler number, the gas is nearly frozen, and for large values it is in thermal equilibrium. At values near unity, the vibrational temperature lags behind the translational-rotational temperature but is dynamic enough to non-negligibly impact the behavior of the flow [112],[150]. The often-employed non-dimensional quantities of M and Re are also important here. As a sample single-mode visualization is given in Fig. 7.1.

In order to extract the entropy production values for each simulation without lengthy postprocessing, routines were added to TWRBLES that calculate and output the entropy production terms at each point. The contribution of each point is then added to form single values for the entropy generation due to viscous dissipation, internal heat conduction, and relaxation (for TWRBLES). Conduction includes both conduction along the vibrational and translational-rotational temperature gradients. In addition, the entropy generation from the inviscid flux, which accounts for the entropy generation in the implicit subgrid model, i.e., numerical dissipation, was calculated. This allowed for the relative comparison of the entropy generation modes across a variety of conditions.

7.1.1 Initial Conditions and Critical Parameters

A Taylor-Green vortex is a simple case of an isotropic turbulence, which has been studied extensively as a first-analysis for turbulence simulations. Unfortunately, the definition of the Taylor-Green vortex becomes unclear at high Mach number. The Taylor-Green initial condition assigns a single Fourier mode of velocity to the velocity field in two dimensions, and then solves a pressure Poisson equation to calculate the pressure field. When compressibility is considered, the flow may be assumed initially isentropic, which yields negative density at high Mach number, or isothermal, which yields extremely large pressures and densities. Samtaney [114] found these problems in analysis of isotropic turbulence as well, and so proposed a simpler initial condition in which all three thermodynamic properties (pressure, density, and temperature) are constant. This was found by that author to be significantly more robust with respect to increasing Mach number, and to not have significant impact on the resultant turbulent decay of quantities relative to their initial values. It was also confirmed by Peng and Yang that initial thermodynamic condition did not have a significant impact on the decay of turbulent kinetic energy in a Taylor-Green vortex [115]. For this study, most of the cases examined use a single mode with constant initial thermodynamic

properties. A sample case is also run with the temperature and density derived from the ideal gas law given the pressure Poisson in order investigate the importance of the initial condition to the thermodynamic portion of the entropy generation to ensure the findings from this section are valid in general. The initial conditions for the pressure-Poisson Taylor-Green case are given by

$$\begin{aligned}
u &= V_0 \sin\left(\frac{x}{L}\right) \cos\left(\frac{y}{L}\right) \cos\left(\frac{z}{L}\right) \\
v &= -V_0 \cos\left(\frac{x}{L}\right) \sin\left(\frac{y}{L}\right) \cos\left(\frac{z}{L}\right) \\
w &= 0 \\
p &= p_0 + \frac{\rho_0 V_0^2}{16} \left(\cos\left(\frac{2x}{L}\right) + \cos\left(\frac{2y}{L}\right) + \cos\left(\frac{2z}{L}\right) + 2 \right)
\end{aligned} \tag{7.10}$$

where $\rho_0 = 1$, $p_0 = \frac{1}{\gamma}$, and V_0 is the turbulent Mach number per the nondimensionalized variable definitions.

The use of γ for the case with vibrational nonequilibrium should be addressed as well. For this analysis, γ is the ratio of the translational rotational enthalpy to energy, irrespective of the vibrational component. The initial conditions are calculated with a vibrationally frozen assumption, and all parts of the solver take into account the fact that γ no longer describes the complete thermodynamic properties of the simulation, as is the case for calorically perfect behavior. Because the solver individually treats translational-rotational energy, for which C_v and C_p actually are constant, and vibration, for which energy capacity is a function of temperature, there is no need for a "variable γ ." Variable total specific heats are necessary for cases which include vibrational energy storage but assume it to always be in equilibrium with other modes, so the overall heat capacity changes as the vibrational energy capacity does [149].

For isotropic turbulence cases, the flow was initialized with a sum of Fourier modes in velocity with random orientations, weighted such that a specified wave number is

most energetic [151]. The thermodynamic quantities of these cases are all set to constant values at the initial conditions.

Examination of the vibrational entropy generation term suggests that this term is likely to be very small across a wide variety of conditions. The vibrational entropy variable, being a difference of reciprocals of temperatures, is smaller than the simple temperature reciprocal which premultiplies the viscous dissipation for cases where the temperatures are similar; however, there are examples in the literature of differences between translational-rotational and vibrational temperature which are greater than the vibrational temperature itself, such as the study on a hypersonic double cone conducted by Kieweg et al. [152]. In that simulation, it was found that in some regions of the flow such as inside shockwaves, the vibrational temperature was much smaller than the translational temperature. These differences were greater than 10,000 K in magnitude. At other locations such as in the flow downstream of the SWBLI, the vibrational temperature was greater than the translational temperature by up to 2900 K.

A sample entropy profile for a vibrationally unexcited case is shown in Fig. 7.2. This shows the basic characteristics of the entropy budgets, variations of which will be found in all the cases analyzed here. Early in the simulation, the interactions between shocklets create strong temperature gradients and quickly feed energy from the kinematics of the flow to the translational and rotational energy modes. At this time, the peak thermal nonequilibrium is achieved and cases with appreciable vibrational entropy see that mechanism excited at the same time. These shocklets reflect and interact again, losing some energy to thermal modes with each interaction. This energy transfer sustains the internal temperature gradients and therefore the heat flux entropy generation. Eventually, the shocklets lose enough energy that shocklet interactions are no longer possible and the energy decays by the usual processes of near-incompressible turbulence. This is seen in the entropy budgets as the decline of the entropy generation rates from all modes.

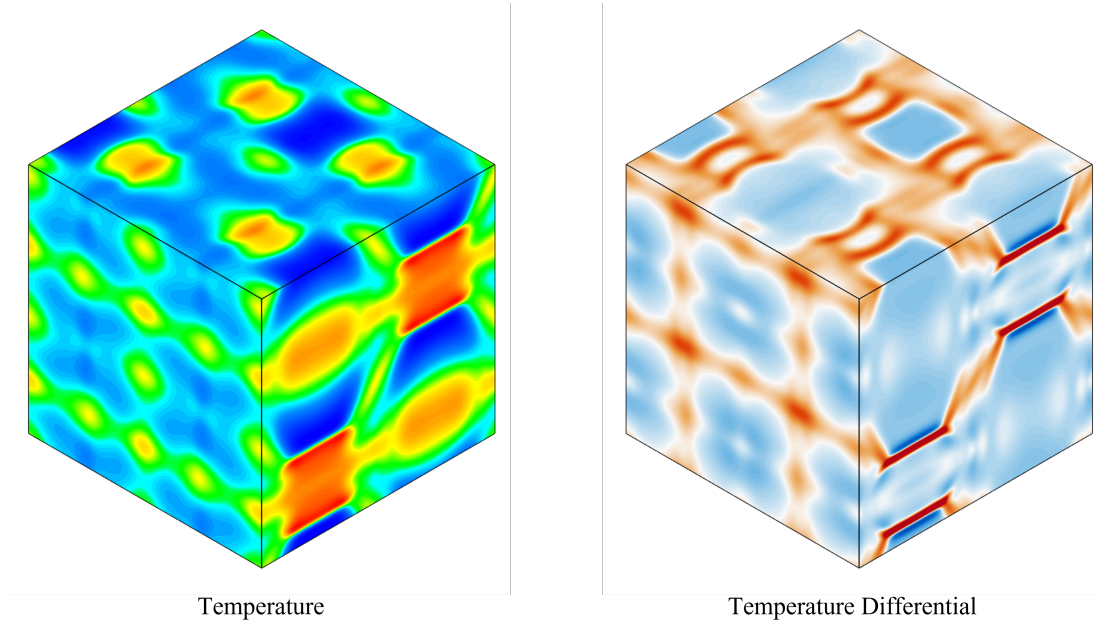


Figure 7.1: Sample snapshot of a compressible single-mode perturbation in vibrational nonequilibrium.

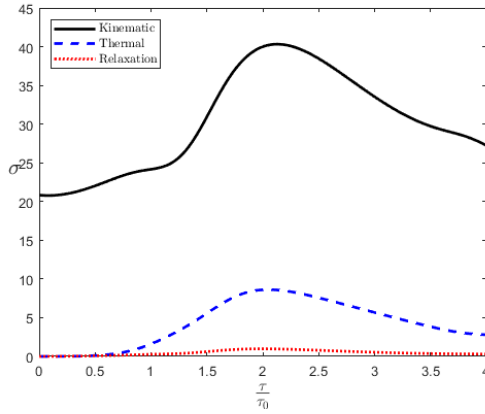


Figure 7.2: Example of the characteristic entropy generation profile for a case with high turbulent Mach number and vibrational excitation

7.1.2 Grid Refinement Study

Being an ILES simulation, it was known ahead of time that some portion of turbulent dissipation would be approximated by numerical dissipation of subgrid scales. This is true for all simulations except for full direct numerical simulation, which resolves all turbulent scales. Nevertheless, the impact of this anticipated phenomena must be quantified so that the other results may be examined in their proper context. Ideally, the inviscid entropy contribution should be as small as possible, with a contribution of zero corresponding to true DNS. There is no universally agreed-upon threshold for what portion of the turbulent dissipation must be resolved in LES beyond the goal of minimization. The primary concern is the numerical dissipation required to resolve shockwaves, which are present for large eddy Mach numbers. Investigation of the inviscid entropy production was done in TWRBLES using three levels of grid refinement, 193^3 , 256^3 , and 332^3 . The grid refinement study was performed at two conditions. The first was a Mach number of 0.5, a unit Reynolds number of 72, and Ψ of 1. This run was aimed at ensuring the solver was deterministically converging as the grid was refined. The second case was run using a Mach number of 1, a Θ of 1.2, a Taylor Reynolds number of 100, and a Ψ of 1. The second grid refinement study is primarily interested in the shocklet interaction region, where the numerical dissipation is critical in resolving the sharp temperature and density gradients during this region. The case chosen to evaluate the the behavior of the shock capturing in flows where it is a critical feature. It also represents one of the more extreme cases examined in this study, and convergence of the cases here indicates that high-quality solutions will be achieved for the other simulations.

For the grid refinement case, the subgrid entropy does not rise above 2.5% of the total entropy generation for any of the cases in the grid refinement study. It is also be observed that most of the entropy that is generated by the subgrid dissipation is resolved as kinematic dissipation for higher levels of grid resolution. While all three grids are consistent with the entropy generation goals, it was found in the case of

the coarsest grid that some undesirable oscillations were found in the entropy values that result directly from the under-resolution of the shocklets. Nevertheless, as seen in Fig. the entropy production values do show some divergence in the presence of strong shocks, but the entropy values re-converge after the strongest shocks have passed. The extra dissipation caused by grid coarseness is energetically recovered as temperature and therefore induces an increase in the local temperature. This increase in turn introduces some spurious relaxation entropy generation, but the value of this spurious generation is much lower than the values observed when the relaxation mode is excited.

7.2 Single-Mode Disturbances

7.2.1 Effect of Mach Number

While the impact of vibrational nonequilibrium has been emphasized to this point, it is critical to note that compressible turbulence analysis has, in general, focused on studying the decay of turbulent kinetic energy in flows. This is a hold-over from incompressible turbulence theory where, as discussed in prior sections, the losses in kinetic energy are actually irrecoverable and thus a complete description of the flow losses. For compressible flows, energy in the flow can be rendered unable to drive further kinematics through conduction of heat as well as kinematic processes. The entropy generation from this mechanism is represented by group 7 of Eq. 4.7. Turbulent kinetic energy budgeting omits this loss mechanism and therefore cannot provide a complete picture of the dynamics of the flow. In order to examine the impact of this mechanism on the overall entropy generation, simulations were run code at a Re_λ of 100 at a sweep of Mach number from 0.1 to 1. It can clearly be seen that the entropy generation from thermal conduction is a significant portion of the overall entropy generation in the domain. This is particularly true early in the simulation as this is when the strongest shocklet interactions happen. During

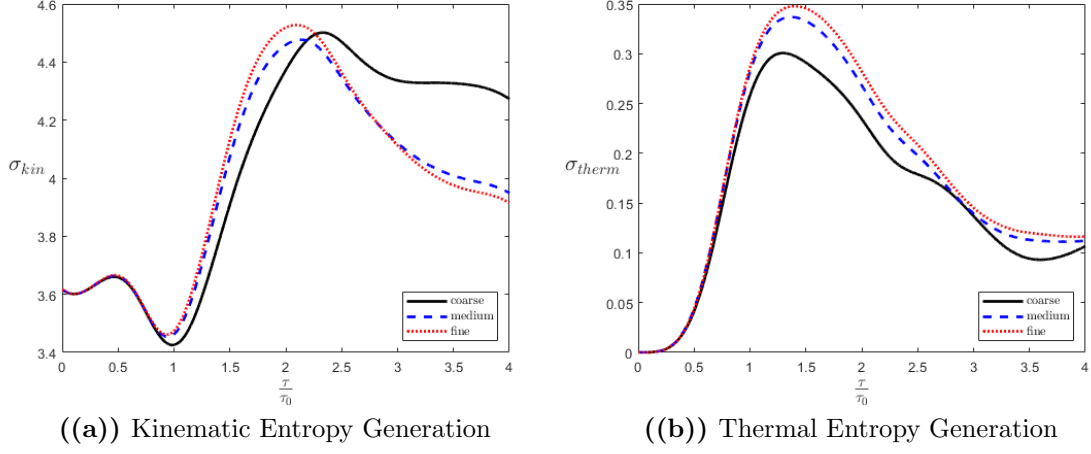


Figure 7.3: Grid convergence of the kinematic and thermal entropy generation terms

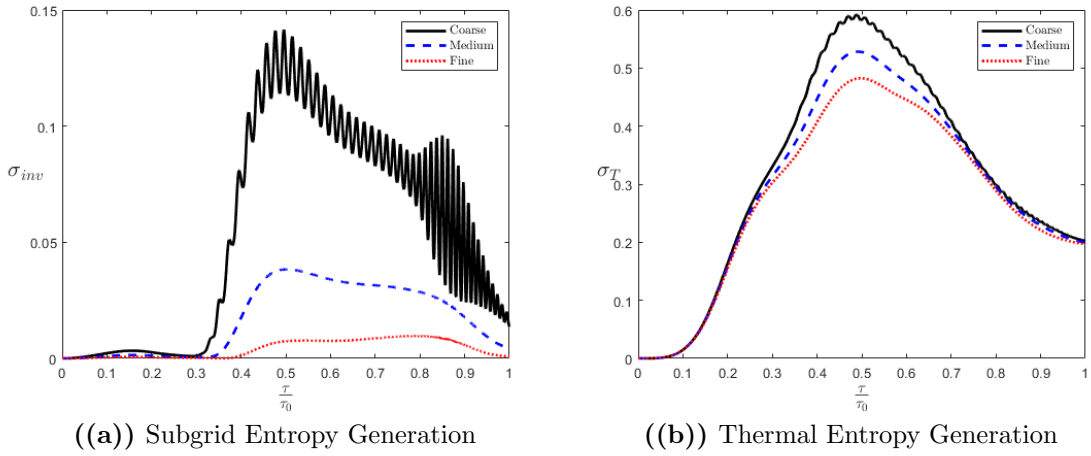


Figure 7.4: Grid convergence of the inviscid and thermal contributions of the entropy generation for the grid refinement test case

these shocklet interactions for the Mach 1 case, the entropy generation by heat conduction reaches nearly 23% of the total entropy production. This is by no means a trivial contribution, nor is the roughly 8% of the total which is contributed by heat conduction after most of the initial shocklets have decayed. As seen in other flow scenarios examined in previous chapters, thermal contributions approach zero as the Mach number drops to zero, demonstrating that the energy methods commonly employed for incompressible flows are valid for that flow regime but not necessarily for higher speeds. It is also once again observed that entropy analysis converges with energy-based methods at incompressible conditions because it accurately captures the decay of the thermal contributions towards zero.

7.2.2 Effect of Relaxation Time

The relationship between the vibrational entropy generation and the relaxation time is somewhat nuanced. Investigating the definition of relaxation entropy reveals that the entropy generation is inversely proportionate to the relaxation time. Physically, this is because entropy is generated by the decay of energy gradients, and the longer the relaxation time, the slower the energy gradient decays and thus the slower entropy is generated. However, the relaxation time is also a critical parameter in the establishment of nonequilibrium in the first place. If the relaxation process proceeds quickly enough, the flow remains in or very near equilibrium. In this case, though the value of τ may be small, the difference between the actual vibrational energy and the equilibrium energy, as well as the difference in the reciprocals of temperatures, will approach zero. In the case of near-equilibrium, the entropy generation of the relaxation process approaches zero. In the other extreme, when the flow is frozen or near-frozen, the vibrational relaxation time is very large. The temperature difference and the energy difference will be large as well, but these values are limited to the case where all of the internal energy is stored in the translational rotational mode. In this limit the temperature and energy differences are still finite, but the relaxation time of

a near-frozen flow approaches infinity, so the entropy generation is zero. Physically, this is the case where no energy transfer happens, so no entropy is generated by the decay of an energy gradient. In the intermediate regime, the entropy generation of the relaxation term is positive. The theoretical maximum entropy generation resulting from these two competing trends is specific to the gas and the time scales of the other present phenomena, but it can be qualitatively understood that relaxation times which promote a balance of appreciable energy differences and non-negligible energy relaxation will be the most entropic.

The dependence on the relaxation time can be examined by varying the vibrational Damköhler number, which can be accomplished either by changing the vibrational relaxation time or the characteristic kinematic time scale, i.e. Mach number, of the flow. For these cases, this was accomplished by increasing the relaxation time parameter. This was chosen because increasing the Mach number also increases the strength of the shocklets in the initial turbulent flow which would place a practical limit on the study where the shocklets stiffen the equation too much and the timestep and grid refinement requirements become prohibitive. Each of these cases was run with a Mach number 1, a Taylor-scale Reynolds number of 105, and a vibrational excitability of 6, ensuring that the vibrational mode was excited throughout the domain. This is an extreme case, but as seen in Ref. [152], flows where the static temperature is much larger than the vibrational excitation temperature of the gas are possible in practical applications. This is particularly true for space applications, where some destinations will have atmospheres consisting of CO_2 , which is much more prone to vibrational excitation than Nitrogen or Oxygen and which has multiple vibrational storage modes. Fig. 7.7 shows a snapshot of the flows analyzed here on a computational mesh size of 256^3 with a non-dimensional time step of 0.0001.

The importance of entropy generation from nonequilibrium can be directly evaluated by examining the portion of the total viscous entropy generation that process represents as the vibrational Damköhler changes number. This has been done, and the results of such an analysis are shown in Fig. 7.19. This figure immediately

shows that the vibrational nonequilibrium contribution can be non-negligible. For the case of $\Theta = 0.01$ the vibrational portion of the entropy generation accounts for slightly more than 5% of the total. While the value of Θ for this case is small, it is observed that the defined time scale may not non-dimensionalized the flow in the best way. The Damköhler number describes the relationship between large eddy turn-over and vibrational relaxation. However, the non-relaxation process which directly competes for the redistribution of energy is actually the conduction of heat away from the shocklet regions, not the large-eddy turn over. Even in the vibrationally excited case, shocklets are required in the flow to introduce a sufficient degree of nonequilibrium that relaxation is on the order of other energy transfer mechanisms.

An interesting result is found in examining the relative contributions of the thermal contribution in the cases with an and without significant relaxation entropy. One might expect that, as relaxation competes directly with heat conduction as a relief mechanism for the temperature gradients introduced by shocklets, cases with vibrational relaxation would have proportionately less thermal entropy. This, however, is not found to be the case. For the case where 5% of the entropy is generated from relaxation, the thermal contribution only decreases by approximately 1.5% of the total, with the majority of the proportional decrease being experienced by the kinematic entropy generation. The apparent mechanism behind this is the relative inability of flows with slower relaxation to mitigate spikes in translational-rotational temperature caused by shocklets. In the cases where vibration responds quickly, the peak translational-rotational temperature inside the shocklets is lower because a portion of that thermal energy has already been stored in the vibrational mode. Because shocklets are a localized phenomena that fill only a portion of the domain, the spikes in temperature they cause introduce strong temperature gradients. With slow relaxation, these storage mechanisms are not available and so these temperature spikes and subsequent temperature gradients are even stronger. Slow relaxation therefore not only increases the entropy generated by the relaxation process itself, but forces more energy to be transferred via conduction, thus largely maintaining the

entropy production of the conductive mode. Neville [112] noted that a properly tuned relaxation time can act as a damper on thermal fluctuations. The relaxation process can be thought of as a non-ideal capacitor for thermal energy, removing it temporarily from the system and then returning it, with each transaction incurring some loss in usable energy. The relaxation time is, both in analogy and in practice, the resistance to this energy exchange, and as ought to be expected increased resistance is observed here to cause more entropy generation. A side-effect of the increased temperature gradients in cases with slow relaxation is increased reliance on numerical dissipation in the inviscid fluxes to resolve the shocklets, the case with $\Theta = 0.01$ experienced a roughly 3% increase in the inviscid entropy generation, which was observed to likely be the result of the slightly stronger shockwaves in that case. Mach 1 turbulence begins to approach the limit where finer grids are required to resolve features for this implementation of TWRBLES in the benchmarking investigation, and so it is not surprising that the code would be sensitive to the relaxation parameters. Nonetheless, the results of this study are consistent with theory and the calculated inviscid entropy remained below the threshold for consideration established earlier throughout the domain.

It might be suspected that the introduction of thermal nonequilibrium presents a problem for the strong Reynolds analogy often utilized in the analysis of compressible turbulence. Because variation in the relaxation time provides a set of cases with identical input parameters but different relaxation entropy generation and vibrational temperature history. Figure 7.9 demonstrates that the velocity-driven kinematic entropy and the thermally-driven thermal entropy scale together regardless of the influence of vibrational temperature.

7.2.3 Effect of Vibrational Excitation Temperature

The influence of the degree of vibrational excitation can be interrogated by varying the characteristic vibrational excitation temperature. For these cases, single-mode

perturbations were analyzed at Mach 0.8, a Taylor microscale Reynolds number of 72, and a Θ of 1. Vibrational excitability was varied by changing the characteristic vibrational excitation temperature. In this study, one run was conducted with the vibrational excitability was less than one, and one run was conducted with vibrational excitability significantly greater than one. The other two runs were intermediate values. The results of this analysis are shown in Fig. 7.10. As can be seen, three of the cases exhibit the expected reduction in vibrationl excitation with reduced Ψ , with the notable exception of the $\Psi = 1.67$ case. This case shows a number of unexpected behaviors compared to the others. The time at which the thermal and vibrational entropy contributions peak is lagged compared to the other cases and decays more slowly. It also does not lie along the trend found in the other cases. This result is found to consistently arise for the conditions run, and so the result appears to be physical. However, the mechanism behind its deviation from the expected results is not known at this time.

The results here are not unexpected in that decreasing the characteristic vibrational temperature increases the vibrational energy capacity, so a constant initial static temperature corresponds to increasing internal energy in the flow

7.2.4 Effect of Taylor-Scale Reynolds Number

Reynolds number sensitivity should be examined in any novel aerodynamic analysis because Reynolds number is a critical nondimensional description of every flow. In order to examine the dependence of the entropy production on Reynolds number, a set of single-mode simulations was run with a turbulent Mach number of 0.8, a Θ of 0.1, a Ψ of 1.05. Taylor-scale Reynolds numbers of 50, 75, and 100. These values were chosen because of how commonly these values are examined in the literature. These values do introduce shocklets to the flow but do not significantly excite the vibrational mode, at least compared to the cases run specifically to examine the vibrational entropy's sensitivity to relaxation parameters. The results of this analysis

are shown in Fig. 7.11, and it is observed that there appears to be a straightforward linear relationship between Reynolds number and the importance of thermal and vibrational entropy generation. This appears to be most pronounced in the large eddy decay where shocklet interactions dominate the flow, after which the entropy generations in each case converge back to similar relative importance. It should be noted that the analysis being undertaken here is that of a decay process, so the specified Reynolds number is only descriptive of the initial flow field, and the velocity field will decay to uniformly zero after sufficient time, at which point the Reynolds number is also zero. The influence of the initial Reynolds number seems to be chiefly felt in the strength of shocklets, since higher Reynolds number corresponds to a less-damped velocity field at the time when the initial counter-flowing fluid structures collide.

This finding is also important to note because Reynolds number is one of the limiting parameters in this study. In some cases, the Reynolds numbers examined have been restricted to values lower than those which would be seen in applications, and the findings here indicate that these cases will under-estimate the relative importance of the non-kinematic entropy generation mechanism as it will behave in application, but that the trends found there are otherwise identical to the application-Reynolds-number case.

7.2.5 Summary of Single-Mode Findings

Taken in sum, the findings from analysis of the decay of single-mode perturbations show several key findings. The first is the apparent existence of a turbulent Mach number threshold above which shocklet interactions become a critical mechanism in the decay of large eddies. This threshold appears to be approximately $M_T = 0.5$. At turbulent Mach numbers greater than this, the flow is initialized with counter-flowing fluid elements whose relative Mach number is greater than 1. It is anticipated that the threshold for shocklet dominance will be slightly higher for

isotropic turbulence because the random distribution of mode orientations requires a higher Mach number to achieve this same effect. Above this threshold, the relative importance of thermal dissipation mechanisms rises quickly. This poses a potential challenge to the applicability of the strong Reynolds analogy for flows at very high Mach number. The available literature suggests that state-of-the-art analysis of turbulent boundary layers through DNS or experiment have begun to approach this limit. These findings are consistent with the results of Zhang, Duan, and Choudhari [83], who found that, for free-stream Mach numbers corresponding to supersonic RMS Mach numbers, the flow experiences significant localized temperature fluctuations, pressure dilatation which in turn produce entropy. The existence of shocklets in the flow is also found to be a prerequisite for appreciable relaxation entropy generation.

The entropy in the domain for a Mach 1 perturbation is shown in Fig. 7.12 as a function of time, and is seen to monotonically increase and asymptotically approach its maximum value. This is in contrast with turbulent kinetic energy, which is decreasing for most, but not all, of the domain. Monotonicity in the total entropy has already been observed in every case up to this point, as every term in every entropy budget has been strictly non-negative for all times.

The value of the relaxational entropy production is found to be strongly dependent on the value of the characteristic relaxation time, with longer times yielding significantly greater entropy generation through this mechanism. The presence or absence of relaxation entropy was found to have no impact whatsoever on the ratio of thermal to kinematic entropy generation. This is in spite of the different distributions of thermal energy between the translational-rotational and vibrational modes. This finding does support the continued use of compressibility transformations for cases in thermal nonequilibrium. It also demonstrates that conservation of energy is an inherent part of the entropy budget equations. Additionally, vibrational entropy appears to be relevant in the temperature range where the vibrational energy mode is fully excited, and dependence of the vibrational energy on temperature is linear.

Reynolds number was found to have a predictable impact on the relative importance of entropy production mechanisms in the flow, and flows with lower-than-application Reynolds numbers can be expected based on these findings to underpredict the importance of thermal entropy generation mechanisms. This is consistent with theory and provides a means of intelligently extrapolating results to even more computation-hostile conditions, which are outside the reliable capabilities of the tools used here.

7.2.6 Influence of Initial Thermodynamic Condition

It has been found in the literature that for Taylor-Green problems, the choice of initial condition for the thermodynamic variables does not significantly impact the kinetic energy decay of the flow [115], [114]. For this study, most cases have used the simplest possible thermodynamic conditions, constant pressure, density, and temperature. This was chosen because the isotropic turbulence cases which the Taylor-Green flows are modeling use a constant property initial condition, and introducing additional differences between those cases and the single-mode cases was not desirable. Essentially, the single-mode runs were treated as a special case of isotropic turbulence rather than as an extension of incompressible Taylor-Green vortex. Still, it must be acknowledged that much of the contemporary literature utilizes an isothermal initial condition for which the pressure is calculated from the Poisson equation and the density is calculated with the ideal gas law. It is therefore necessary to evaluate the influence of the chosen initial condition compared to one which is considered more standard specifically for Taylor-Green flows. Comparison of these two initial conditions for a turbulent Mach number of 1, Reynolds number of 100, Psi of 0.5, and Θ of 0.01 is shown in Fig. 7.13. While the constant-property initial condition does predict a higher share of thermal and relaxational entropy, these effects are still very much relevant to the overall entropy generation and display the same trends in both cases.

7.3 Isotropic Turbulence

Having validated the tools to be used and phenomenologically investigated the influence of critical parameters, it is now of interest to examine more realistic isotropic turbulence. This is done according to the formulation used by Samtaney [114]. Neville [112] used a peak wave number of 8, and that has been replicated for realistic turbulence cases here. Compared to the $k_0 = 1$, the multi-mode cases evolve quickly and impose more strain on the solver. This is because these cases have their shocklets spread across numerous smaller interactions rather than a handful of strong interactions, and the smaller Taylor microscale necessitates larger unit Reynolds numbers to achieve comparable Taylor scale Reynolds numbers. Because of this, most fundamental exploration of the response of entropy to various parameters is done using single-mode cases. Realistic turbulence analysis is focused on running specific individual cases to evaluate the relative importance of individual parameters for various representative scenarios. The exception to this is evaluating the influence of initial temperature. The influence of initial temperature was investigated again to ensure the trends found in single-mode cases were applicable to isotropic turbulence. These cases examined a Mach number of 1, a Re_λ of 50, a peak wave number of 8, a Ψ of 1, and a Θ of 0.1. The results of this analysis are shown in Fig. 7.14 and are found to agree closely with the findings from the single-mode analyses. Overall, the strength of the shocklets is slightly lower than for the single-mode case, and the unit Reynolds number was lower, which has already been shown to decrease the share of thermal entropy generation.

From here, a set of representative cases are examined to ensure the trends observed between the single-mode and isotropic turbulence cases are consistent.

7.3.1 Moderate Mach Number Turbulence

Much of the available literature focuses on turbulent Mach numbers in the neighborhood of 0.5. A representative case was run with a turbulent Mach number of 0.5, a

Re_λ of 72, a k_0 of 8, and a Θ of 0.1, and a Ψ of 1.67. These are the approximate conditions that would be experienced by a reusable vehicle. Duan found that a free-stream Mach number of 8 yielded a peak M_t of approximately 0.4 in turbulent DNS calculations of hypersonic boundary layers. The investigation of the importance of thermal effects in this region is valuable, as the strong Reynolds analogy is generally considered to be valid in this region in the literature [83]. Visualization of the flow field is shown in Fig. 7.16, and the entropy generation results are shown in Fig. 7.15. It is observed that the relative importance of temperature spikes early in the run and then decays to a plateau level. After the initial spike, the influence of shockwaves is largely absent from the flow, though density gradients still exist, and all entropy generation modes decay with time. The relative decay rates of the individual modes leads to the relative importance of temperature slowly rising.

7.3.2 Intermediate Mach Number Turbulence

Increasing the Mach number to 1.2 and decreasing Ψ to 0.01, but keeping all other parameters equal ($Re_\lambda = 50$, $\Theta = 1.2$), the influence of vibrational and thermal entropy generation is seen to increase significantly compared to the lower Mach number case. Thermal entropy generation peaks at approximately 10% of the total. As with the single-mode cases, relaxation entropy is found to achieve relevant values as the initial shocklet interactions take place and then the entropy generation through this mechanism decays again afterwards. Entropy plots for this case are shown in Fig. 7.17. As with the previous case, temperature entropy generation decays more slowly than the other two modes, increasing its relative importance over time.

7.3.3 High Mach Number Turbulence

The most computationally challenging case run in this study was a vibrationally excited isotropic turbulence case with an eddy Mach number of 2. This corresponds to a free-stream Mach number in the mid teens [83]. This case was run with a

microscale Reynolds number of 27, which is the lowest of the cases examined here, and a peak wave number of 4 instead of 8. The results of this case are consistent with other findings. Because the vibrational relaxation for this case is faster than the previous one, vibrational nonequilibrium is not able to develop to the degree required to drive significant entropy generation.

7.3.4 Relaxationally Inhibited Turbulence

It was found in the single-mode examination that extended relaxation times are necessary to develop the energy differential which sustains relaxational losses. The extensibility of this to isotropic turbulence was investigated in $M = 0.8$, $Re_\lambda = 50$, $k_o = 8$, $\Psi = 5$, $\Theta = 0.01$ turbulence. This case demonstrates that even for turbulent Mach numbers less than one, vibrational relaxation can be an appreciable source of entropy. Together with the previous case, the necessity of "slow" relaxation time in driving relaxation entropy is made clear.

7.3.5 Summary of Isotropic Turbulence Results

Overall, the isotropic turbulence results obtained support the conclusions drawn from the single perturbation mode analysis. At higher Mach numbers, thermal mechanisms contribute a significant fraction of the overall entropy generation of the system. Vibrational relaxation can contribute a small but non-negligible fraction of the overall entropy generation of the system if the Mach number is high enough to support shocklets and the relaxation time is slow. Isotropic turbulence cases were limited in achievable Reynolds number by the solver, and trends from the single-mode cases suggest that even greater values of thermal entropy generation could be achieved by increasing this parameter.

7.4 Discussion and Conclusions

Taylor-Green-type flows and isotropic turbulence have been analyzed from an entropy perspective. The entropy analysis is able to quantify the relative importance of kinematic and thermal mechanisms in the entropy production of the flows. The entropy generation caused by vibrational relaxation was also calculated. Single-mode perturbation cases are used to evaluate the dependence of the flow on various critical parameters, and the findings from these cases are evaluated for more general applicability through comparison to isotropic turbulence cases.

A critical takeaway from this analysis is the important role that thermal heat transfer plays in the entropy generation of the flow. Examination of the turbulent kinetic energy profile and thermal entropy generation profile together paints a clear picture in which TKE fails to capture thermal losses and erroneously predicts a "reversal" in turbulent decay, whereas entropy accurately captures the regions where thermal entropy generation accounts for a significant fraction of the overall losses while the kinematic portion temporarily slows. Physically, this corresponds to energy being temporarily stored in internal modes by shocklets in the flow. From this, it is clear that entropy is the proper metric for tracking total losses due to turbulence, and this work provides a clear and consistent method for calculating entropy generation.

The role of vibrational relaxation in turbulent entropy generation was also examined. In the absence of a base flow, it is unlikely that the overall contribution of vibrational entropy generation will be greater than a single-digit percentage of the total, but the key factors which influence this contribution are explored. It is found that shocklets are a prerequisite for appreciable vibrational entropy generation, and longer relaxation times in the Landou-Teller model of relaxation yield higher entropy generation. The effect of vibrational relaxation time is found to be significantly greater than the role of characteristic relaxation temperature, even in cases where the static temperature of the flow is much lower than the threshold for full vibrational excitation. This is still of interest for real flows, where a sustained difference

between the mean vibrational and mean translational-rotational temperature may drive significant turbulent relaxational entropy in the right circumstances.

The findings made here support the shift in turbulence analysis from one centered on calculating turbulent kinetic energy to a paradigm centered on entropy. Overall, turbulent kinetic energy does have convenient properties for modeling; it is easy to calculate and its connection to surface stresses is relatively clear. Unfortunately, it is fundamentally incapable of considering all loss mechanisms for highly-compressible flows, and its limitations will be continually exacerbated as analysis and systems design push towards more complex and higher-speed systems. In contrast, entropy is guaranteed by its fundamental definition to be monotonic and fully descriptive of losses in the flow. The challenges associated with turbulence analysis centered on entropy are in calculating the generation rate of entropy and identifying means of modeling design-relevant quantities from it. The first challenge is addressed here in full, and the second challenge is left for the aerodynamics community.

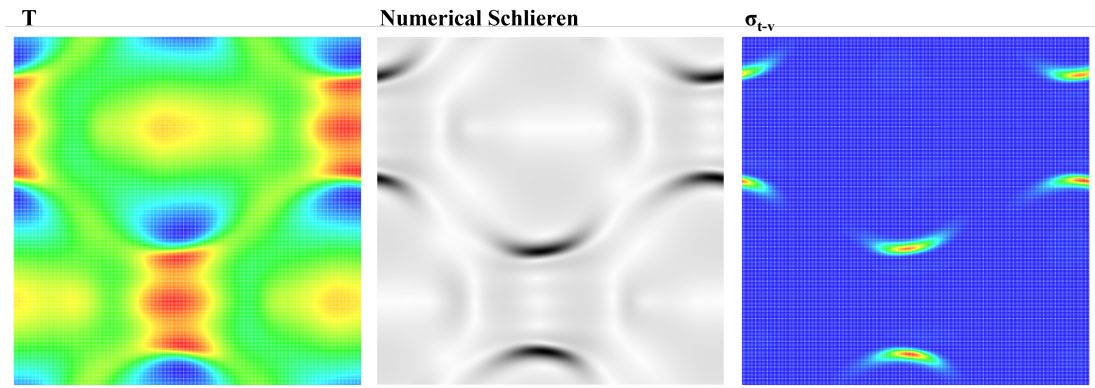


Figure 7.5: Contours of relevant thermal quantities in a characteristic single-mode turbulence simulation showing vibrational entropy generation only occurs in regions of shock-induced thermal nonequilibrium

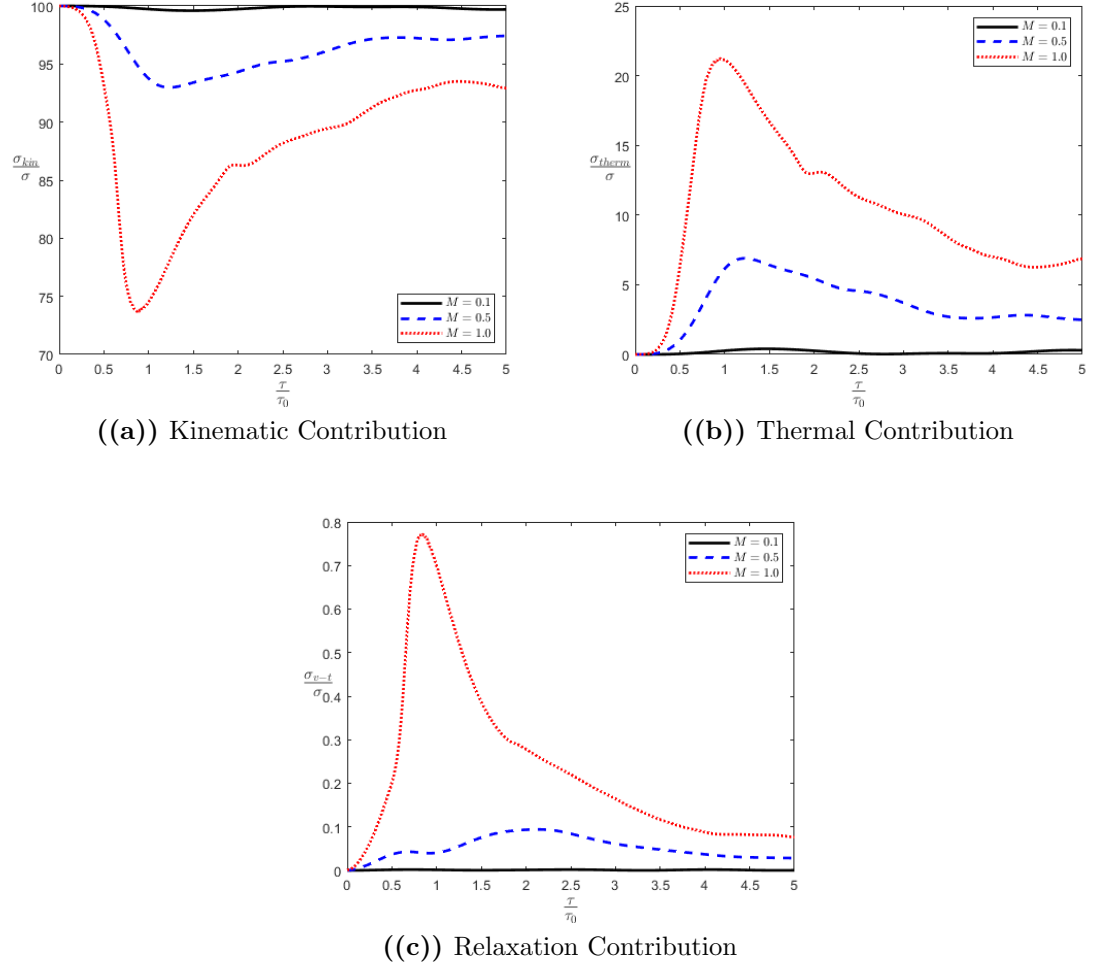


Figure 7.6: Contributions of each RHS entropy generation term as a percentage of the total instantaneous entropy generation

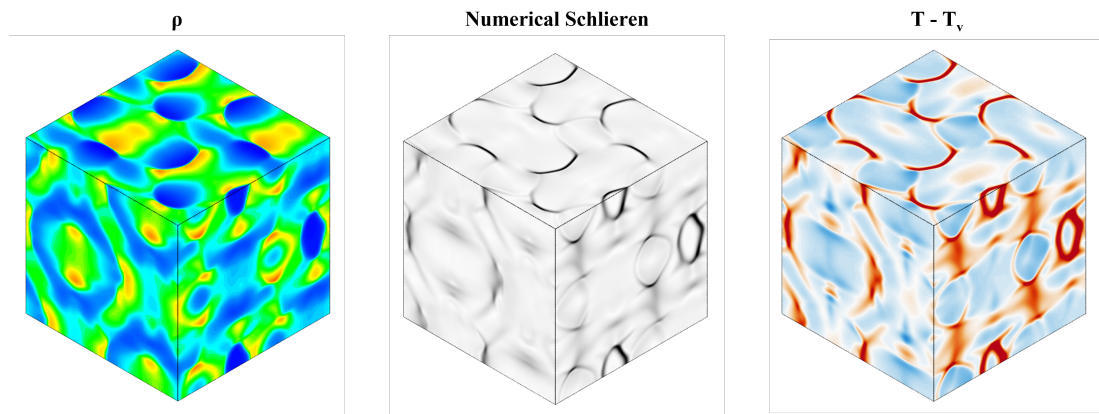


Figure 7.7: Representative visualization of the isotropic turbulent decay examined in this section.

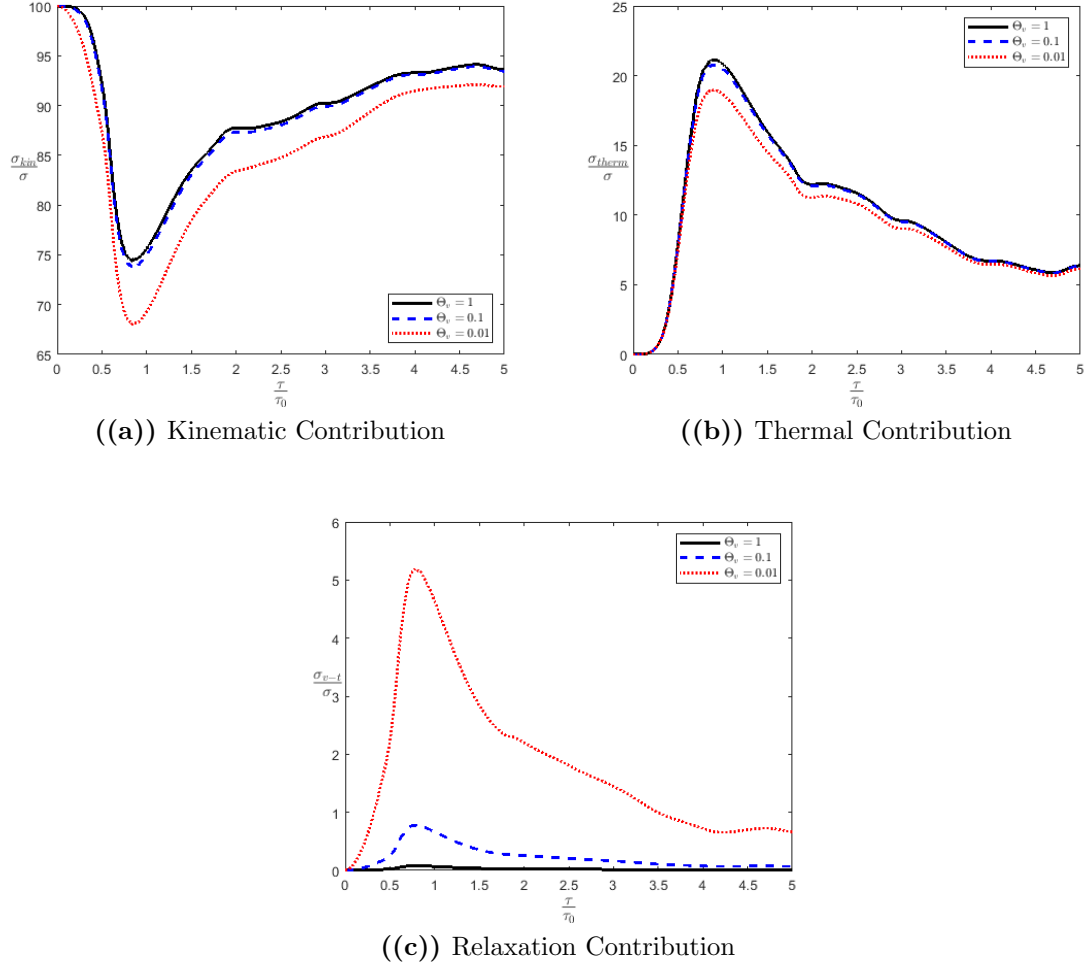


Figure 7.8: Contributions of each RHS entropy generation term as a percentage of the total instantaneous entropy generation

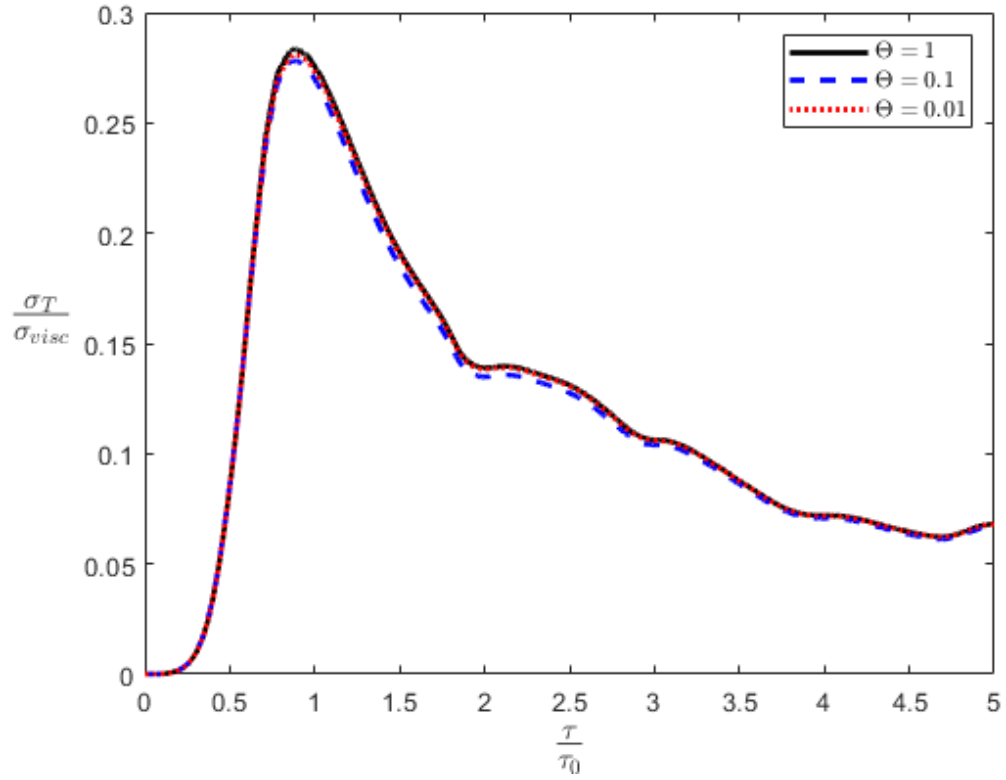


Figure 7.9: Ratio of thermal entropy production to kinematic entropy production for the three cases with different vibrational relaxation times. These cases range in vibrational relaxation entropy generation from negligible contributions to 5% of the total.

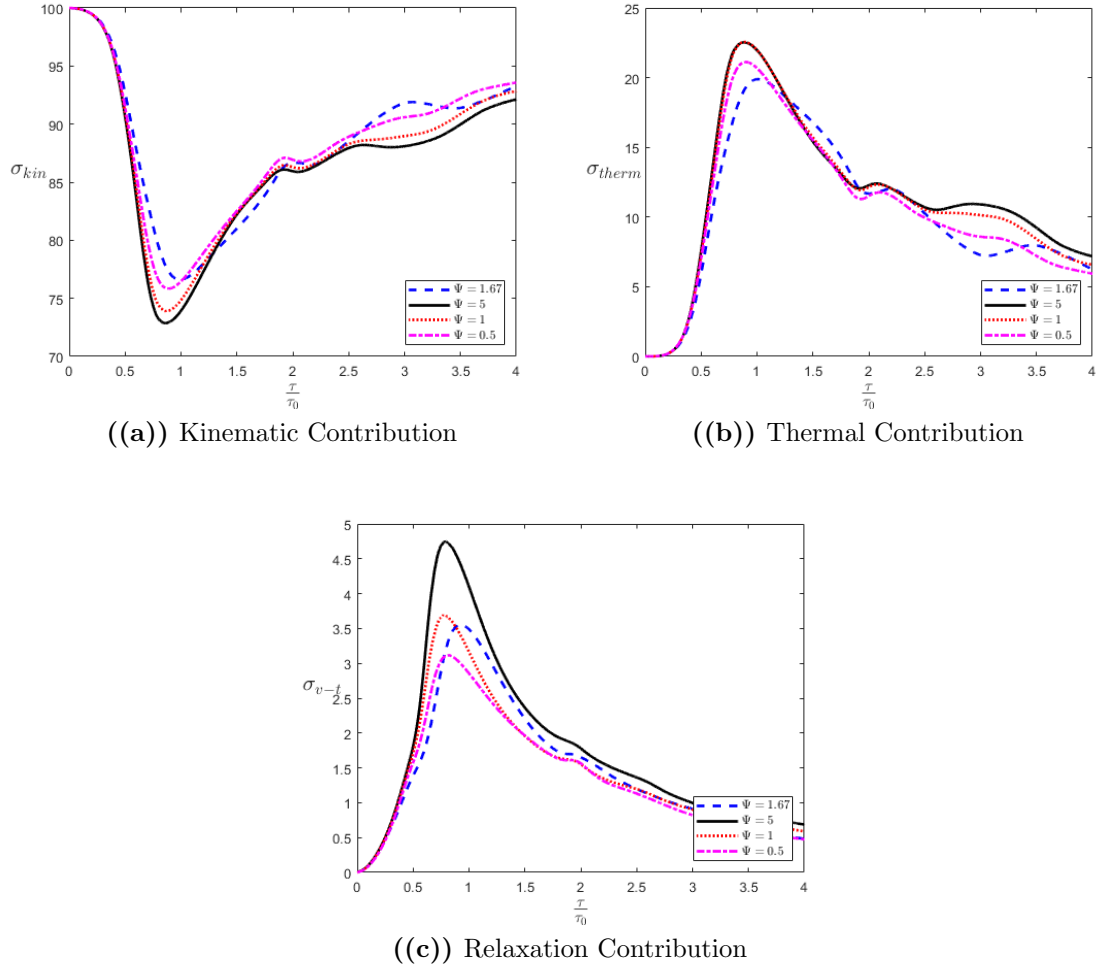


Figure 7.10: Contributions of each RHS entropy generation term as a percentage of the total instantaneous entropy generation

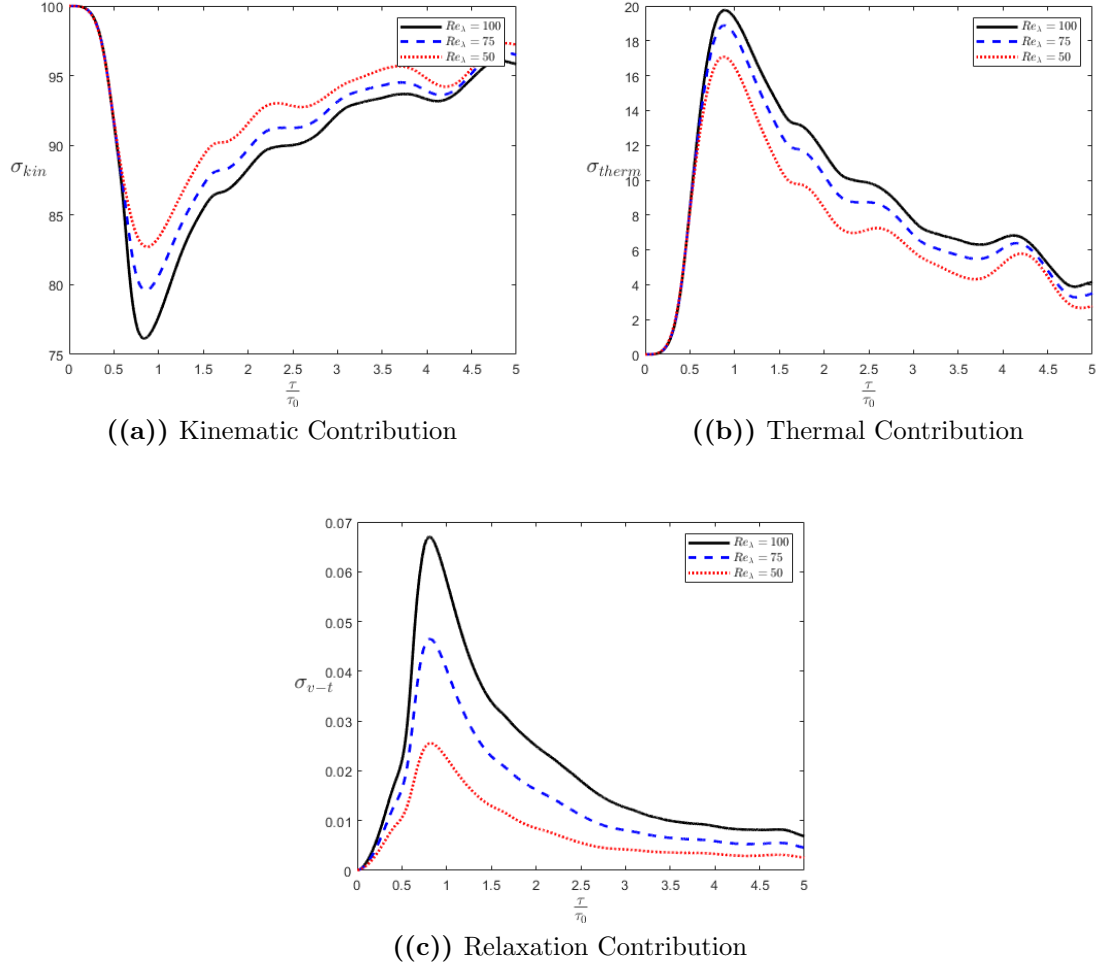


Figure 7.11: Contributions of each RHS entropy generation term as a percentage of the total instantaneous entropy generation

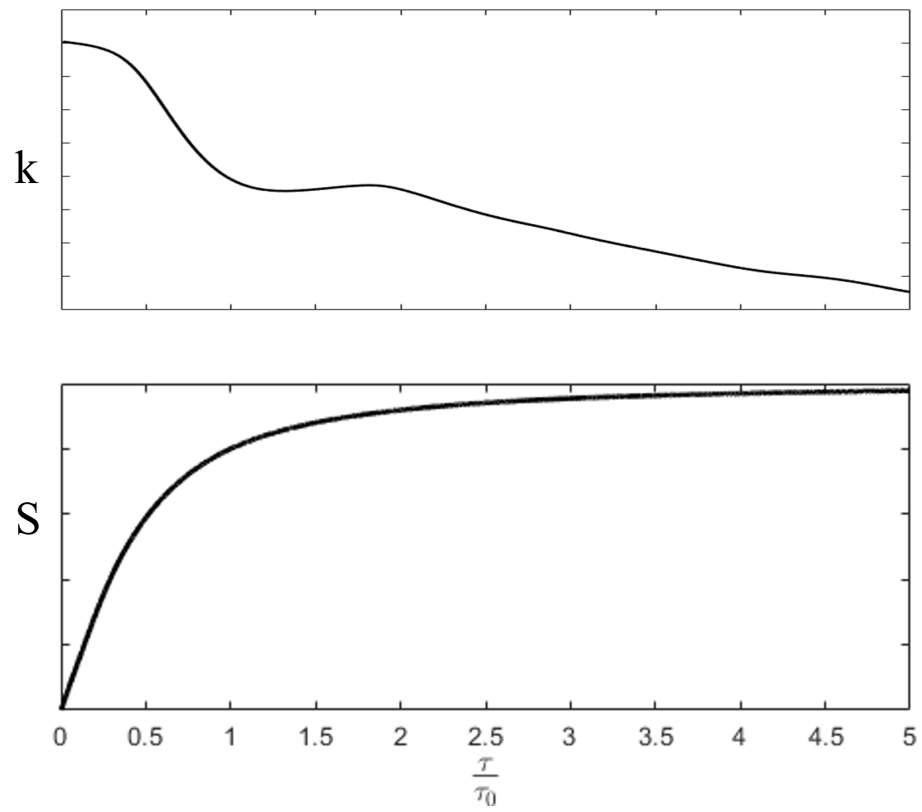


Figure 7.12: Entropy and turbulent kinetic energy for a single-mode case with a turbulent Mach number of 1.

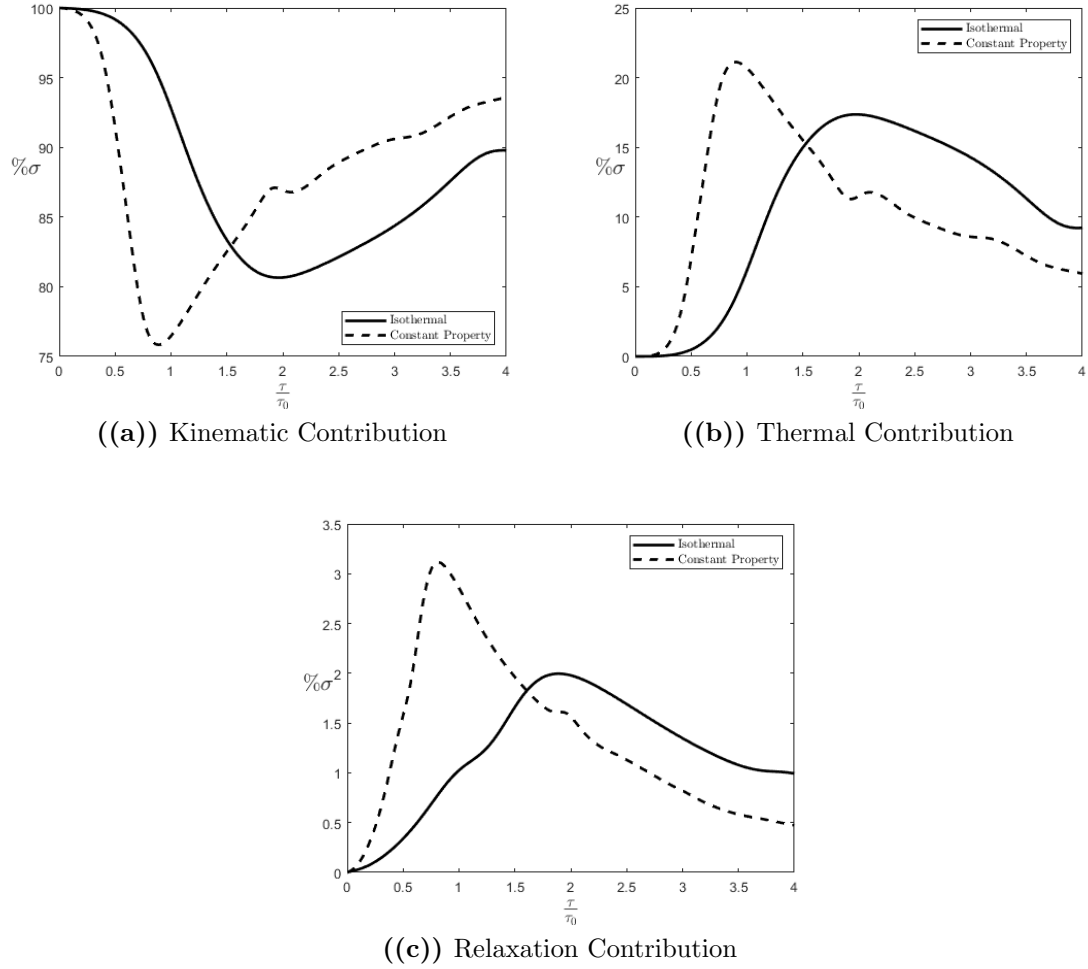


Figure 7.13: Contributions of each RHS entropy generation term as a percentage of the total instantaneous entropy generation for both sets of initial conditions.

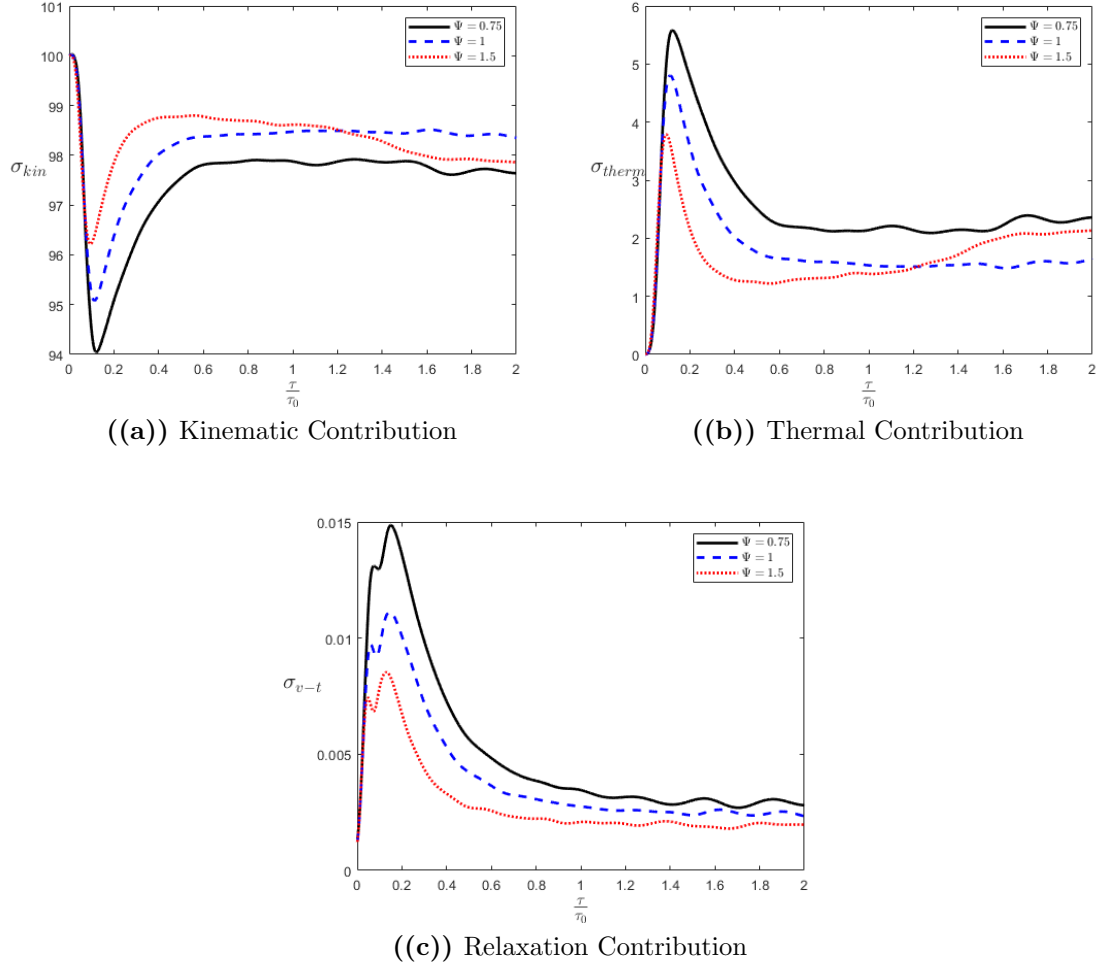


Figure 7.14: Contributions of each RHS entropy generation term as a percentage of the total instantaneous entropy generation

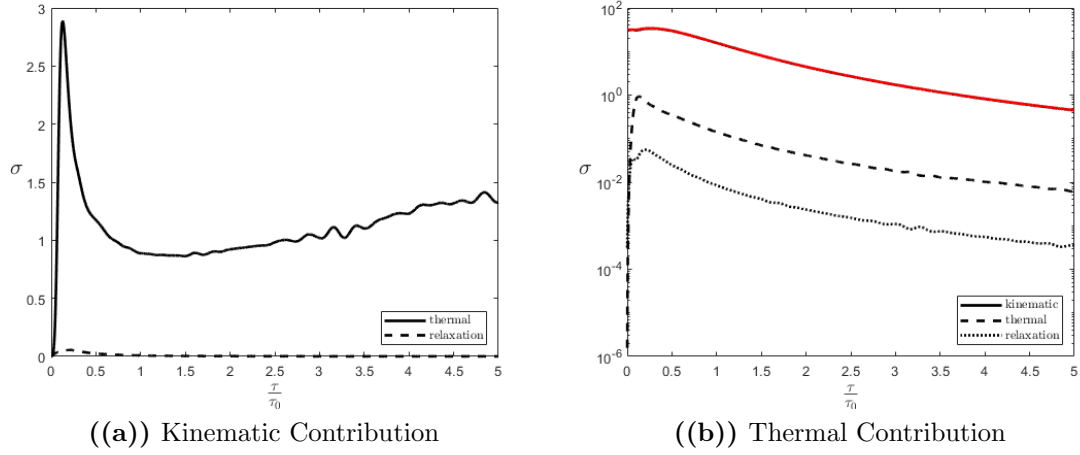


Figure 7.15: Thermal and relaxational entropy rate portions, along with total entropy generation from each mode plotted in log scale

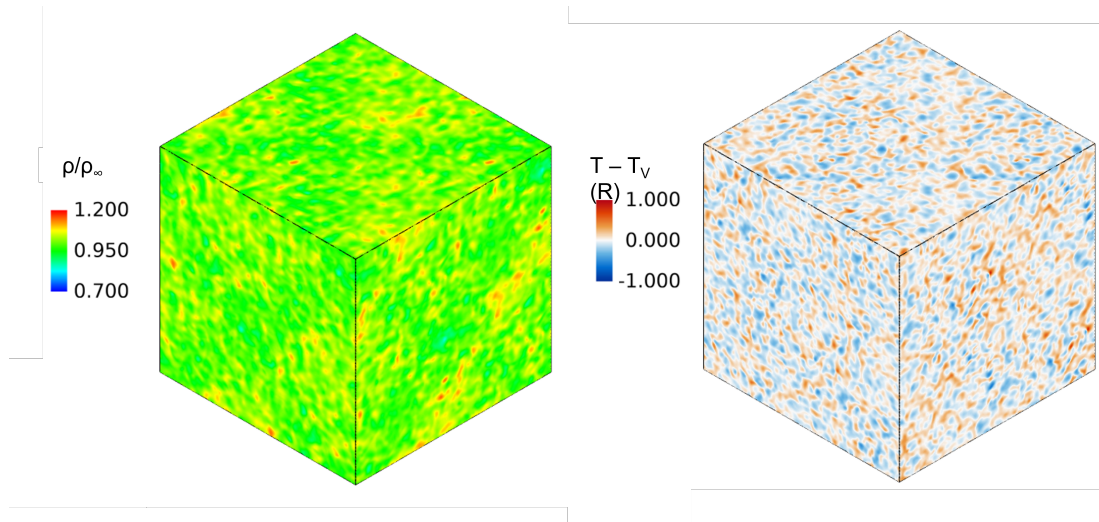


Figure 7.16: Visualization of the $M = 0.5$ isotropic turbulence case showing diffuse but relatively low-magnitude thermal nonequilibrium

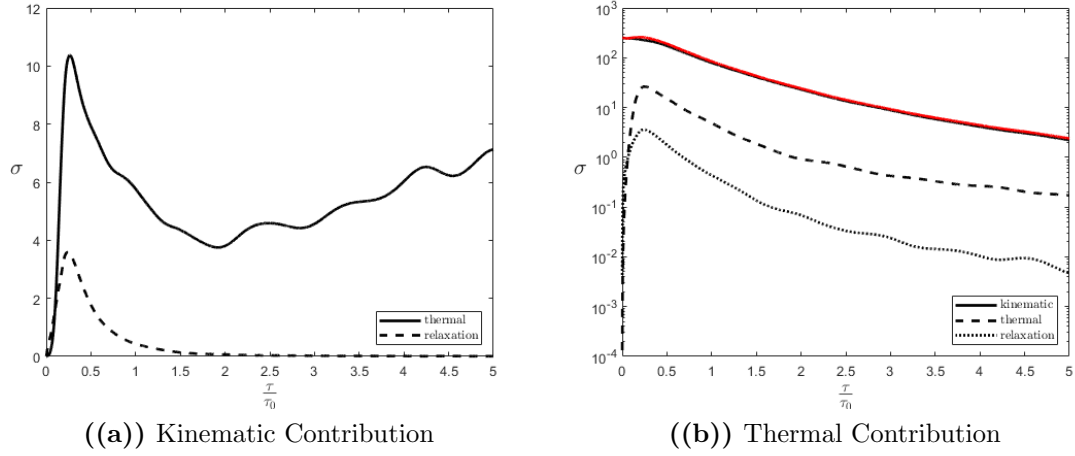


Figure 7.17: Thermal and relaxational entropy rate portions, along with total entropy generation from each mode plotted in log scale

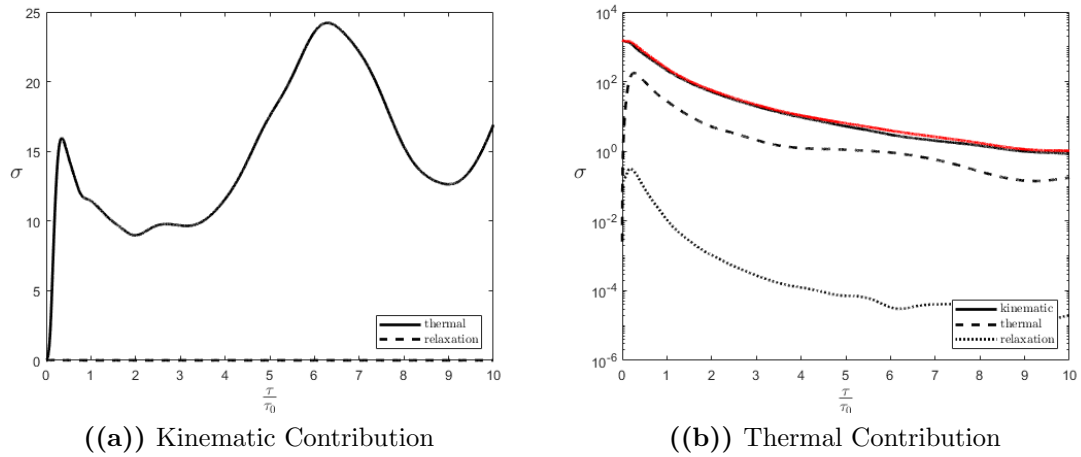
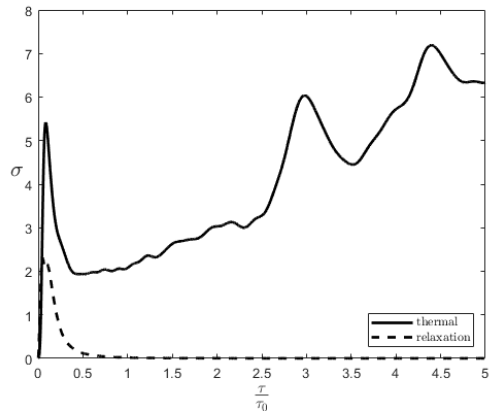
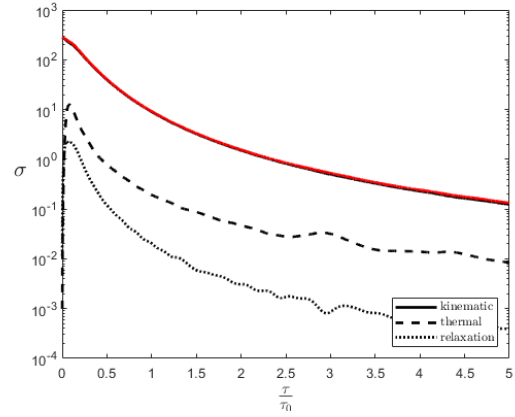


Figure 7.18: Thermal and relaxational entropy rate portions, along with total entropy generation from each mode plotted in log scale



((a)) Kinematic Contribution



((b)) Thermal Contribution

Figure 7.19: Thermal and relaxational entropy rate portions, along with total entropy generation from each mode plotted in log scale

Chapter 8

Conclusions

8.1 Summary of Findings

An entropy normalization for application to generalized compressible fluids problems has been derived from the definition of entropy. This normalization relies on the principles of a mathematical entropy analysis for the Navier-Stokes equations, and uses the most general continuum definition of entropy available. This normalization may be employed for flows with multiple species, thermal imperfection, caloric imperfection, finite-rate reactions, and thermal nonequilibrium. This normalization represents a significant broadening of the varieties of flows which may be meaningfully analyzed through modal decomposition and stability analyses which rely on matrix norms for physical consistency. The generalized norm is found to be diagonal for flows whose perturbations are expressed in the primitive variable set, which reflects the independence of the portions of the molecular partition function and provides computational and practical benefits over a dense normalization.

The entropy normalization is mathematically compared to the Chu norm, and it is found through this comparison that the Chu norm is thermodynamically consistent with the entropy norm as a normalization of heat transfer. This represents an update in the community's understanding of the Chu norm and a reaffirmation of

its validity for applications such as POD. Furthermore, the entropy norm is shown mathematically to converge with the Chu norm for cases with small local temperature gradients, reflecting the relationship between entropy and heat transfer in classical thermodynamics.

Entropy transport is then calculated using the entropy variables developed for the derivation of the norm. Entropy transport attributable to each RHS term of the generalized Navier-Stokes is examined. It is shown that thermal non-equilibrium necessarily produces entropy regardless of the specifics of the nonequilibrium state. The entropy transport is then decomposed for application to turbulent flows. The ability to rigorously calculate entropy generation provides an alternative to energy-based turbulence analysis whose validity is vulnerable to strong compressibility effects.

The entropy normalization is applied in four test scenarios. The first case is transient growth of perturbations in self-similar compressible boundary layers in a calorically and thermally perfect equilibrium gas. This served as a test bed to examine the expectations of the relationship between the new entropy norm and the Chu norm. The convergence of the norms for low-Mach number flows with small temperature gradients was verified, and the two norms were shown to begin to demonstrate differences in predicted mode shapes around the onset of the hypersonic regime. The entropy norm is found to be more sensitive to thermodynamic perturbations in the flow.

The entropy norm is demonstrated for full-scale POD of a three-dimensional time accurate simulation of a jet-in-crossflow. The first iteration of the jet-in-crossflow examines a jet into Mach 4 crossflow whose composition is the same as the free-stream flow. This test case provides a dynamic flow with significant temperature and velocity gradients. In keeping with the trends found in the mathematical and stability analyses, the norms are found to disagree most in regions with very high local temperature gradients. The entropy norm does not demonstrate significantly different distributions of modal dynamic content than the Chu norm, and the dense and

diagonal implementations of the entropy norm demonstrate identical modal dynamic content distributions.

The entropy norm is evaluated for application to higher Reynolds number external aerodynamics flows by examining the application to the cone-slice-ramp, a model developed for examination of compression corner SWBLIs which also includes relevant vortex structures. In the absence of features which directly introduce temperature gradients to the flow, the entropy norm tends place focus on features which include significant temperature gradients, namely shockwaves and viscous phenomena.

The final POD test case is entropy-based POD applied to a multispecies jet in crossflow. This case demonstrates the applicability of entropy-based POD to multispecies flows and the value added by the multispecies analysis. Combined kinematic and diffusive flow features are found to be better examined by the multispecies POD implementation, and no dynamic content distribution disadvantages are introduced by using the multispecies norm.

Entropy analysis is applied to calculate the entropy generation by kinematic, thermal, and relaxational mechanisms in compressible turbulence with vibrational nonequilibrium. Overall, it is found that thermal mechanisms account for a very significant portion of the entropy generation in compressible turbulent flows when turbulent shocklets exist. This mechanism is not accounted for by TKE, leading that quantity to lose monotonicity at high Mach number. Entropy is found to be fully monotonic in all cases, with each source of entropy generation being positive for all time. Vibrational relaxation is found to be an important entropy generation mechanism only for cases with very long relaxation times. Still, the possibility of relevant levels of vibrational relaxation entropy suggests that flows with significant mean-flow thermal nonequilibrium could see this mode as a major mechanism of entropy generation.

Overall the entropy norm presented here has been demonstrated to be effective and practical for examining compressible flows, and much more broadly applicable than the normalization schemes currently in use. Entropy analysis has been demonstrated

both to exceed the capabilities of energy methods at high speeds, and to underpin the capabilities of those methods for incompressible conditions.

8.2 Future Perspectives

This work presents the process of entropy analysis and showcases its applications, but as with any relatively new avenue of research there are many paths which could not be fully explored in this work. This section outlines those avenues which the authors view as most theoretically rich. Each of these potential avenues is likely to lead to even more research questions, and while the author has attempted to limit the scope of this work to those questions specifically relevant for engineering applications, some of them may be of greater interest to related research communities whose focus is more fundamental.

8.2.1 Entropy Solutions to PDEs with Source Terms

In this work, it is assumed that the entropy analysis used for the thermal equilibrium Navier-Stokes equations is a valid template for that of the thermal nonequilibrium case. Because the entropy norm only requires the entropy function to be convex (which it proves to be), this assumption is never fully evaluated. This assumption is necessary because the introduction of thermal nonequilibrium introduces a source term to the governing equations. So far, there is no conclusive proof that entropy solutions for PDE systems with source terms exist. The existence of entropy solutions for ODE's with source terms has been demonstrated with some stipulations on the nature of the source term, but this does not necessarily mean that the same is true of systems of equations, especially in light of the difficulties often associated with calculations of entropy solutions. A mathematical proof of the possible existence of entropy solutions for this type of PDE system would fully unite the mathematical,

thermochemical, and fluid dynamic views on entropy, whose equivalence has been fruitfully presumed but not rigorously proven.

8.2.2 Reduced-Order Models with Multiple Bases

It was discussed in the findings from POD analysis using the entropy and Chu norms that the entropy norm demonstrates greater sensitivity to thermodynamic effects than the Chu norm. In most applications, POD bases for reduced order models are found by performing a single decomposition using a single L^2 norm and therefore a single matrix normalization. However, Lee and Dowell [153] recently demonstrated a method for constructing reduced-order models using two POD bases. Their work, which examined a 2-D incompressible flow, found that reduced-order models constructed with multiple bases have more reliably predictable accuracy than those constructed with either individual basis. While this approach has not yet been applied to compressible flows and likely requires further characterization, it is expected that this approach would synergize well with the entropy norm, which is observed to be particularly capable of capturing thermodynamic phenomena.

8.2.3 Exploration of the Bounds of the Partition Formulation

In this work, entropy can straightforwardly be calculated because the mechanisms of entropy generation are taken to be independent from one another and calculated with their own partition functions. This is, at least implicitly, also an assumption of the thermal nonequilibrium Navier-Stokes. In order for the energy states of each of these modes to be considered separately they must be independent at least to the point that exchange of energy between them may be quantified. This formulation of the entropy terms is valid for an ideal or Van der Waals gas, but may not hold up if further real gas effects are considered. It is also worth considering the value added in exploring the influence of nonequilibrium effects far into the real gas regime, since this analysis ultimately relies on the continuum interpretation of fluids problems

presented by the Navier-Stokes. Applications for which real gas or electromagnetic effects dominate may be better analyzed through another lens. Extension of this type of analysis to a Boltzmann framework rather than a Navier-Stokes framework would enable robust analysis of hybrid CFD-DSMC results which are becoming increasingly available owing to ever-expanding computational capabilities. One aspect of flow dynamics which is not given significant consideration but which is often of interest to the simulation of hypersonic vehicle systems is material ablation. Ablation presents an entirely new set of physics and challenges to the already complex set of physics to be considered for these flows, hence its exclusion here. Nevertheless, ablation of gases would introduce polyatomic contaminants whose gas properties are significantly different than species normally considered by aerodynamicists, and for which the ideal gas or Van der Waals assumption may be a less appropriate model.

8.2.4 Maturation of TWRBLES

TWRBLES, the parallelized nonequilibrium Navier-Stokes solver developed for the evaluation of entropy generation in isotropic turbulence, is still embryonic by solver standards. Beyond the obvious improvements, namely implementing more boundary conditions, there are capability upgrades that should be made to the solver. TWRBLES uses Gnoffo's upwinded inviscid flux eigenvectors, and more recent work in the literature provides alternate formulations of the eigenvectors which may improve the capabilities of TWRBLES. Additionally, the original WRBLES solver has received upgrades to its numerical formulation which increased its robustness at higher Mach numbers, and TWRBLES should be similarly upgraded to handle higher Mach and Reynolds numbers. TWRBLES also does not consider all of the nonequilibrium and chemistry effects described in other sections, and it would benefit a more generalized way of handling individual gas properties so that monatomics and polyatomics could be studied. TWRBLES is, in summary, a promising start for a

high-order LES solver for thermal nonequilibrium, but more work is required for the tool to achieve wider utility.

8.2.5 Entropy-Based Turbulence Analysis

Turbulent kinetic energy has been shown here and elsewhere in the literature to not maintain monotonicity in all cases for highly-compressible flows. Many classes of turbulence model rely on tracking TKE, and second-moment turbulence models, which may eventually achieve dominance over first-moment closures, must calculate TKE transport if they are formulated with typical energy arguments. Entropy has been presented as a more robust alternative to TKE for compressible turbulence, and a method of calculating entropy generation by each irreversible process is presented. The next step would therefore be to develop an alternative modeling framework by which unresolved turbulent features could be modeled by predicting entropy generation by those mechanisms using the mean flow properties.

8.3 Concluding Remarks

Entropy is found to be an extremely robust metric for flow analysis with respect to compressibility effects and the numerous physical complications they introduce. The work described here provides a strong theoretical foundation for the development of engineering tools for a variety of purposes. By firm grounding in fundamental physics and broad applicability, entropy analysis can remove uncertainty from the analysis and design process and gives a framework by which fluid dynamics systems of all kinds can be comparably examined. While the fundamental nature of this work leaves many avenues to be explored, there is significant evidence and a wealth of strong theoretical arguments which support not only the continued pursuit of entropy methods, but elucidate the underlying role of entropy in the success of the energy methods it may replace.

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Appendix

Appendix A

Matrix Definitions of Entropy Norm

The matrix Jacobians of the relevant flow variable sets with respect to one another are presented here. These expressions are used to construct S_{qq} , the Hessian of entropy and the entropy normalization. In each of these expressions, subscripts denote the variable set with respect to which the Jacobian derivative is being taken. The definitions of S , entropy, $\mathbf{q}$, the conservative flow variables, and $\mathbf{v}$, the primitive flow variables,

$$S = -\rho s = -\rho \left[\frac{R}{\gamma - 1} \ln \left(\frac{T}{T_\infty} \right) - R \ln \left(\frac{\rho}{\rho_\infty} \right) \right] \quad (\text{A.1})$$

$$\mathbf{q} = [\rho, \rho u, \rho v, \rho w, \rho e_o]^T \quad (\text{A.2})$$

$$\mathbf{v} = [\rho, u, v, w, T]^T \quad (\text{A.3})$$

are based on the ideal gas law and the assumption of a calorically perfect gas. The entropy norm is derived by using the chain rule to piece together the appropriate mappings which will yield the matrix norm. This requires use of 5×5 matrix mappings between variable sets,

$$\frac{\partial S}{\partial v} = S_v = \left(R - s, 0, 0, 0, -\frac{\rho R}{(1 - \gamma)T} \right) \quad (\text{A.4})$$

$$S_q = S_v \mathbf{v}_q = \mathbf{w}^T = \left[C_p - s - \frac{u^2 + v^2 + w^2}{2T}, \frac{u}{T}, \frac{v}{T}, \frac{w}{T}, -\frac{1}{T} \right] \quad (\text{A.5})$$

where

$$\mathbf{v}_q = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{v_1}{\rho} & \frac{1}{\rho} & 0 & 0 & 0 \\ -\frac{v_2}{\rho} & 0 & \frac{1}{\rho} & 0 & 0 \\ -\frac{v_3}{\rho} & 0 & 0 & \frac{1}{\rho} & 0 \\ \frac{(\gamma-1)(2RT+v_1^2+v_2^2+v_3^2-2h)}{2R\rho} & -\frac{(\gamma-1)v_1}{R\rho} & -\frac{(\gamma-1)v_2}{R\rho} & -\frac{(\gamma-1)v_3}{R\rho} & \frac{\gamma-1}{R\rho} \end{bmatrix} \quad (\text{A.6})$$

Given the entropy variables, $\mathbf{w}$, the same process can be used to differentiate again with respect to $\mathbf{q}$, yielding the desired mapping, S_{qq} . This mapping requires a differentiation of the entropy variables,

$$S_{qq} = \mathbf{w}_q = \mathbf{w}_v \mathbf{v}_q \quad (\text{A.7})$$

where

$$\mathbf{w}_v = \begin{bmatrix} \frac{R}{\rho} & -\frac{u_1}{T} & -\frac{u_2}{T} & -\frac{u_3}{T} & \frac{R}{T} + \frac{u_1^2}{2T^2} + \frac{u_2^2}{2T^2} + \frac{u_3^2}{2T^2} - \frac{h}{T^2} \\ 0 & \frac{1}{T} & 0 & 0 & -\frac{u_1}{T^2} \\ 0 & 0 & \frac{1}{T} & 0 & -\frac{u_2}{T^2} \\ 0 & 0 & 0 & \frac{1}{T} & -\frac{u_3}{T^2} \\ 0 & 0 & 0 & 0 & \frac{1}{T^2} \end{bmatrix} \quad (\text{A.8})$$

Appendix B

Turbulent Entropy Transport

B.1 Enthalpy Diffusion

$$\begin{aligned}
\sigma_h \approx & \sum_k^{e,v,tr} \sum_s^{all} -\frac{\rho'}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) + \frac{\bar{\rho} T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) + \frac{\rho' T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) \\
& -\frac{\bar{\rho}}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) - \frac{\rho'}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(h_k'' D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) + \frac{\bar{\rho} T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(h_k'' D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) + \frac{\rho' T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(h_k'' D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) \\
& -\frac{\bar{\rho}}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(h_k'' D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) - \frac{\rho'}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(h_k'' D_s \frac{\partial}{\partial x_j} y'_s \right) + \frac{\bar{\rho} T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(h_k'' D_s \frac{\partial}{\partial x_j} y'_s \right) + \frac{\rho' T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(h_k'' D_s \frac{\partial}{\partial x_j} y'_s \right) \quad (B.1) \\
& -\frac{\bar{\rho}}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(h_k'' D_s \frac{\partial}{\partial x_j} y'_s \right) - \frac{\rho'}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} y'_s \right) + \frac{\bar{\rho} T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} y'_s \right) + \frac{\rho' T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} y'_s \right) \\
& -\frac{\bar{\rho}}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} y'_s \right)
\end{aligned}$$

$$\begin{aligned}
\bar{\sigma}_h \approx & \sum_k^{e,v,tr} \sum_s^{all} -\frac{\bar{\rho}}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(\tilde{h}_k D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) - \frac{\rho'}{\tilde{T}_k} \frac{\partial}{\partial x_j} \left(C_{p,k} T_k'' D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) \\
& + \frac{\bar{\rho} T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(C_{p,k} T_k'' D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) + \frac{\rho' T_k''}{\tilde{T}_k^2} \frac{\partial}{\partial x_j} \left(C_{p,k} T_k'' D_s \frac{\partial}{\partial x_j} \tilde{y}_s \right) \quad (B.2)
\end{aligned}$$

B.2 Species Continuity

$$\begin{aligned}
\sigma_c \approx & \sum_{all} -\frac{\bar{u}_i \bar{u}_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) - \frac{2\bar{u}_i u'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) - \\
& \frac{u'_i u'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) + \frac{T' \bar{u}_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) + \\
& \frac{2T' u'_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) + \frac{T'_i u'_i u'_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) - \bar{s} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) \\
& - s' \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) - \frac{\bar{u}_i \bar{u}_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) \\
& - \frac{2\bar{u}_i u'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) - \frac{u'_i u'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) + \frac{T' \bar{u}_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) \\
& \frac{2T' u'_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) + \frac{T'_i u'_i u'_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) - \bar{s} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) - s' \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) \\
& - \frac{2\bar{u}_i u'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} y'_s) - \frac{u'_i u'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} y'_s) + \frac{T' \bar{u}_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} y'_s) \\
& + \frac{2T' u'_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} y'_s) + \frac{T'_i u'_i u'_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} y'_s) - \bar{s} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} y'_s) - s' \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} y'_s) \quad (B.3) \\
& - \frac{\bar{u}_i \bar{u}_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} y'_s) - \frac{2\bar{u}_i u'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) - \frac{u'_i u'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) + \frac{T' \bar{u}_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) \\
& + \frac{2T' u'_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) + \frac{T'_i u'_i u'_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) - \bar{s} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) - s' \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) - \\
& - \frac{\bar{u}_i \bar{u}_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) - \frac{\bar{u}_i \bar{u}_i}{\bar{T}} \bar{w} - \frac{2\bar{u}_i u'_i}{\bar{T}} \bar{w} - \frac{u'_i u'_i}{\bar{T}} \bar{w} + \frac{T' \bar{u}_i \bar{u}_i}{\bar{T}^2} \bar{w} + \frac{2T' u'_i \bar{u}_i}{\bar{T}^2} \bar{w} + \frac{T'_i u'_i u'_i}{\bar{T}^2} \bar{w} - \bar{s} \bar{w} - s' \bar{w} \\
& - \frac{\bar{u}_i \bar{u}_i}{\bar{T}} \dot{w}' - \frac{2\bar{u}_i u'_i}{\bar{T}} \dot{w}' - \frac{u'_i u'_i}{\bar{T}} \dot{w}' + \frac{T' \bar{u}_i \bar{u}_i}{\bar{T}^2} \dot{w}' + \frac{2T' u'_i \bar{u}_i}{\bar{T}^2} \dot{w}' + \frac{T'_i u'_i u'_i}{\bar{T}^2} \dot{w}' - \bar{s} \dot{w}' - s' \dot{w}' \\
& + \bar{w} \frac{\bar{h}_{s,tr}}{\bar{T}} + \bar{w} \frac{C_{p,s,tr} T'}{\bar{T}} - \bar{w} \frac{\bar{h}_{s,tr} T'}{\bar{T}^2} - \bar{w} \frac{C_{p,s,tr} T'^2}{\bar{T}^2} + \dot{w}' \frac{\bar{h}_{s,tr}}{\bar{T}} + \dot{w}' \frac{C_{p,s,tr} T'}{\bar{T}} - \dot{w}' \frac{\bar{h}_{s,tr} T'}{\bar{T}^2} - \dot{w}' \frac{C_{p,s,tr} T'^2}{\bar{T}^2} \\
& + \bar{w} \frac{\bar{h}_{s,v}}{\bar{T}_v} + \bar{w} \frac{C_{p,s,v} T'_v}{\bar{T}_v} - \bar{w} \frac{\bar{h}_{s,v} T'_v}{\bar{T}_v^2} - \bar{w} \frac{C_{p,s,v} T_v'^2}{\bar{T}_v^2} + \dot{w}' \frac{\bar{h}_{s,v}}{\bar{T}_v} + \dot{w}' \frac{C_{p,s,v} T'_v}{\bar{T}_v} - \dot{w}' \frac{\bar{h}_{s,v} T'_v}{\bar{T}_v^2} - \dot{w}' \frac{C_{p,s,v} T_v'^2}{\bar{T}_v^2} \\
& + \bar{w} \frac{\bar{h}_{s,e}}{\bar{T}_e} + \bar{w} \frac{C_{p,s,e} T'_e}{\bar{T}_e} - \bar{w} \frac{\bar{h}_{s,e} T'_e}{\bar{T}_e^2} - \bar{w} \frac{C_{p,s,e} T_e'^2}{\bar{T}_e^2} + \dot{w}' \frac{\bar{h}_{s,e}}{\bar{T}_e} + \dot{w}' \frac{C_{p,s,e} T'_e}{\bar{T}_e} - \dot{w}' \frac{\bar{h}_{s,e} T'_e}{\bar{T}_e^2} - \dot{w}' \frac{C_{p,s,e} T_e'^2}{\bar{T}_e^2}
\end{aligned}$$

$$\begin{aligned}
\bar{\sigma}_c \approx & \sum_{all} -\frac{\bar{u}_i \bar{u}_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) - \frac{\bar{u}'_i \bar{u}'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) \\
& + \frac{2\bar{T}' \bar{u}'_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) + \frac{\bar{T}'_i \bar{u}'_i \bar{u}'_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) - \bar{s} \frac{\partial}{\partial x_j} (D_s \bar{\rho} \frac{\partial}{\partial x_j} \bar{y}_s) \\
& - \frac{2\bar{u}_i \bar{u}'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) - \frac{\bar{u}'_i \bar{u}'_i}{\bar{T}} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) + \frac{\bar{T}' \bar{u}_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) \\
& + \frac{2\bar{T}' \bar{u}'_i \bar{u}_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) + \frac{\bar{T}'_i \bar{u}'_i \bar{u}'_i}{\bar{T}^2} \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) - \bar{s}' \frac{\partial}{\partial x_j} (D_s \rho' \frac{\partial}{\partial x_j} \bar{y}_s) \\
& \frac{\bar{u}_i \bar{u}_i}{\bar{T}} \bar{\dot{w}} - \frac{\bar{u}'_i \bar{u}'_i}{\bar{T}} \bar{\dot{w}} - \frac{2\bar{T}' \bar{u}'_i \bar{u}_i}{\bar{T}^2} \bar{\dot{w}} + \frac{\bar{T}'_i \bar{u}'_i \bar{u}'_i}{\bar{T}^2} \bar{\dot{w}} - \bar{s} \bar{\dot{w}} + \bar{\dot{w}} \frac{\bar{h}_{s,tr}}{\bar{T}} - \bar{\dot{w}} \frac{C_{p,s,tr} \bar{T}^{r2}}{\bar{T}^2} \\
& + \bar{\dot{w}} \frac{\bar{h}_{s,v}}{\bar{T}_v} - \bar{\dot{w}} \frac{C_{p,s,v} \bar{T}_v^{r2}}{\bar{T}_v^2} + \bar{\dot{w}} \frac{\bar{h}_{s,e}}{\bar{T}_e} - \bar{\dot{w}} \frac{C_{p,s,e} \bar{T}_e^{r2}}{\bar{T}_e^2}
\end{aligned} \tag{B.4}$$

B.3 Viscous Dissipation

$$\begin{aligned}
\sigma_{visc} \approx & \frac{1}{\bar{T}} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} + \frac{1}{\bar{T}} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}'_j}{\partial x_i} + \frac{1}{\bar{T}} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} + \frac{1}{\bar{T}} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}'_j}{\partial x_i} - \\
& \frac{\bar{T}'}{\bar{T}^2} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} - \frac{\bar{T}'}{\bar{T}^2} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}'_j}{\partial x_i} - \frac{\bar{T}'}{\bar{T}^2} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} - \frac{\bar{T}'}{\bar{T}^2} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}'_j}{\partial x_i} - \\
& \frac{2}{3\bar{T}} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_k}{\partial x_k} - \frac{2}{3\bar{T}} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}'_k}{\partial x_k} - \frac{2}{3\bar{T}} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}_k}{\partial x_k} - \frac{2}{3\bar{T}} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}'_k}{\partial x_k} + \\
& \frac{2\bar{T}'}{3\bar{T}^2} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_k}{\partial x_k} + \frac{2\bar{T}'}{3\bar{T}^2} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}'_k}{\partial x_k} + \frac{2\bar{T}''}{3\bar{T}^2} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}_k}{\partial x_k} + \frac{2\bar{T}'}{3\bar{T}^2} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}'_k}{\partial x_k} + \\
& \frac{1}{\bar{T}} \left(\frac{\partial \bar{u}_i}{\partial x_j} \right)^2 + \frac{1}{\bar{T}} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j} + \frac{1}{\bar{T}} \left(\frac{\partial \bar{u}'_i}{\partial x_j} \right)^2 - \frac{\bar{T}'}{\bar{T}^2} \left(\frac{\partial \bar{u}_i}{\partial x_j} \right)^2 - \frac{\bar{T}'}{\bar{T}^2} \frac{\partial \bar{u}'_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j} - \frac{\bar{T}'}{\bar{T}^2} \left(\frac{\partial \bar{u}'_i}{\partial x_j} \right)^2
\end{aligned} \tag{B.5}$$

$$\begin{aligned}
\bar{\sigma}_{visc} \approx & \frac{1}{\bar{T}} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} + \frac{1}{\bar{T}} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_i} - \frac{T'}{\bar{T}^2} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial u'_j}{\partial x_i} - \frac{T'}{\bar{T}^2} \frac{\partial u'_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_i} - \frac{T'}{\bar{T}^2} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_i} - \\
& \frac{2}{3\bar{T}} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_k}{\partial x_k} - \frac{2}{3\bar{T}} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_k}{\partial x_k} + \frac{2T'}{3\bar{T}^2} \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial u'_k}{\partial x_k} + \frac{2T'}{3\bar{T}^2} \frac{\partial u'_i}{\partial x_j} \frac{\partial \bar{u}_k}{\partial x_k} + \frac{2T'}{3\bar{T}^2} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_k}{\partial x_k} + \\
& \frac{1}{\bar{T}} \left(\frac{\partial \bar{u}_i}{\partial x_j} \right)^2 + \frac{1}{\bar{T}} \left(\frac{\partial u'_i}{\partial x_j} \right)^2 - \frac{T'}{\bar{T}^2} \frac{\partial u'_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j} - \frac{T'}{\bar{T}^2} \left(\frac{\partial u'_i}{\partial x_j} \right)^2
\end{aligned} \tag{B.6}$$

B.4 Vibrational and Electronic Relaxation

$$\begin{aligned}
\sigma_{v-t} \approx & \frac{\bar{\rho}_s \bar{e}_v^*}{\bar{T} \tau_{v-t}} - \frac{\bar{\rho}_s \bar{e}_v}{\bar{T} \tau_{v-t}} + \frac{\bar{\rho}_s e_v^{*'}}{\bar{T} \tau_{v-t}} - \frac{\bar{\rho}_s e_v'}{\bar{T} \tau_{v-t}} + \frac{\rho'_s \bar{e}_v^*}{\bar{T} \tau_{v-t}} - \frac{\rho'_s \bar{e}_v}{\bar{T} \tau_{v-t}} + \frac{\rho'_s e_v^{*'}}{\bar{T}} - \frac{\rho'_s e_v'}{\bar{T} \tau_{v-t}} \\
& - \frac{\bar{\rho}_s \bar{e}_v^*}{\bar{T}_v \tau_{v-t}} + \frac{\bar{\rho}_s \bar{e}_v}{\bar{T}_v \tau_{v-t}} - \frac{\bar{\rho}_s e_v^{*'}}{\bar{T}_v \tau_{v-t}} + \frac{\bar{\rho}_s e_v'}{\bar{T}_v \tau_{v-t}} - \frac{\rho'_s \bar{e}_v^*}{\bar{T}_v \tau_{v-t}} + \frac{\rho'_s \bar{e}_v}{\bar{T}_v \tau_{v-t}} - \frac{\rho'_s e_v^{*'}}{\bar{T}_v \tau_{v-t}} + \frac{\rho'_s e_v'}{\bar{T}_v \tau_{v-t}} \\
& - \frac{T' \bar{\rho}_s \bar{e}_v^*}{\bar{T}^2 \tau_{v-t}} + \frac{T' \bar{\rho}_s \bar{e}_v}{\bar{T}^2 \tau_{v-t}} - \frac{T' \bar{\rho}_s e_v^{*'}}{\bar{T}^2 \tau_{v-t}} + \frac{T' \bar{\rho}_s e_v'}{\bar{T}^2 \tau_{v-t}} - \frac{T' \rho'_s \bar{e}_v^*}{\bar{T}^2 \tau_{v-t}} + \frac{T' \rho'_s \bar{e}_v}{\bar{T}^2 \tau_{v-t}} - \frac{T' \rho'_s e_v^{*'}}{\bar{T}^2 \tau_{v-t}} + \frac{T' \rho'_s e_v'}{\bar{T}^2 \tau_{v-t}} \\
& + \frac{T'_v \bar{\rho}_s \bar{e}_v^*}{\bar{T}_v^2 \tau_{v-t}} - \frac{T'_v \bar{\rho}_s \bar{e}_v}{\bar{T}_v^2 \tau_{v-t}} + \frac{T'_v \bar{\rho}_s e_v^{*'}}{\bar{T}_v^2 \tau_{v-t}} - \frac{T'_v \bar{\rho}_s e_v'}{\bar{T}_v^2 \tau_{v-t}} + \frac{T'_v \rho'_s \bar{e}_v^*}{\bar{T}_v^2 \tau_{v-t}} - \frac{T'_v \rho'_s \bar{e}_v}{\bar{T}_v^2 \tau_{v-t}} + \frac{T'_v \rho'_s e_v^{*'}}{\bar{T}_v^2 \tau_{v-t}} - \frac{T'_v \rho'_s e_v'}{\bar{T}_v^2 \tau_{v-t}}
\end{aligned} \tag{B.7}$$

$$\begin{aligned}
\bar{\sigma}_{v-t} \approx & \frac{\bar{\rho}_s \bar{e}_v^*}{\bar{T} \tau_{v-t}} - \frac{\bar{\rho}_s \bar{e}_v}{\bar{T} \tau_{v-t}} + \frac{\bar{\rho}'_s e_v^{*'}}{\bar{T} \tau_{v-t}} - \frac{\bar{\rho}'_s e_v'}{\bar{T} \tau_{v-t}} - \frac{\bar{\rho}_s \bar{e}_v^*}{\bar{T}_v \tau_{v-t}} + \frac{\bar{\rho}_s \bar{e}_v}{\bar{T}_v \tau_{v-t}} - \frac{\bar{\rho}'_s e_v^{*'}}{\bar{T}_v \tau_{v-t}} + \frac{\bar{\rho}'_s e_v'}{\bar{T}_v \tau_{v-t}} \\
& - \frac{\bar{\rho}_s \bar{T}' e_v^{*'}}{\bar{T}^2 \tau_{v-t}} + \frac{\bar{\rho}_s \bar{T}' e_v'}{\bar{T}^2 \tau_{v-t}} - \frac{\bar{T}' \rho'_s \bar{e}_v^*}{\bar{T}^2 \tau_{v-t}} + \frac{\bar{T}' \rho'_s \bar{e}_v}{\bar{T}^2 \tau_{v-t}} - \frac{\bar{T}' \rho'_s e_v^{*'}}{\bar{T}^2 \tau_{v-t}} + \frac{\bar{T}' \rho'_s e_v'}{\bar{T}^2 \tau_{v-t}} \\
& + \frac{\bar{\rho}_s \bar{e}_v^{*'} \bar{T}'_v}{\bar{T}_v^2 \tau_{v-t}} - \frac{\bar{\rho}_s \bar{e}_v' \bar{T}'_v}{\bar{T}_v^2 \tau_{v-t}} + \frac{\bar{T}'_v \rho'_s \bar{e}_v^*}{\bar{T}_v^2 \tau_{v-t}} - \frac{\bar{T}'_v \rho'_s \bar{e}_v}{\bar{T}_v^2 \tau_{v-t}} + \frac{\bar{T}'_v \rho'_s e_v^{*'}}{\bar{T}_v^2 \tau_{v-t}} - \frac{\bar{T}'_v \rho'_s e_v'}{\bar{T}_v^2 \tau_{v-t}}
\end{aligned} \tag{B.8}$$

$$\begin{aligned}
\sigma_{v-e} \approx & \frac{\bar{\rho}_s \bar{e}_v^*}{\bar{T}_e \tau_{v-e}} - \frac{\bar{\rho}_s \bar{e}_v}{\bar{T}_e \tau_{v-e}} + \frac{\bar{\rho}_s e_v^{**'}}{\bar{T}_e \tau_{v-e}} - \frac{\bar{\rho}_s e'_v}{\bar{T}_e \tau_{v-e}} + \frac{\rho'_s \bar{e}_v^{**}}{\bar{T}_e \tau_{v-e}} - \frac{\rho'_s \bar{e}_v}{\bar{T}_e \tau_{v-e}} + \frac{\rho'_s e_v^{*'}}{\bar{T}_e} - \frac{\rho'_s e'_v}{\bar{T}_e \tau_{v-e}} \\
& - \frac{\bar{\rho}_s \bar{e}_v^{**}}{\bar{T}_v \tau_{v-e}} + \frac{\bar{\rho}_s \bar{e}_v}{\bar{T}_v} - \frac{\bar{\rho}_s e_v^{*'}}{\bar{T}_v \tau_{v-e}} + \frac{\bar{\rho}_s e'_v}{\bar{T}_v \tau_{v-e}} - \frac{\rho'_s \bar{e}_v^{**}}{\bar{T}_v \tau_{v-e}} + \frac{\rho'_s \bar{e}_v}{\bar{T}_v \tau_{v-e}} - \frac{\rho'_s e_v^{*'}}{\bar{T}_v \tau_{v-e}} + \frac{\rho'_s e'_v}{\bar{T}_v \tau_{v-e}} \\
& - \frac{T'_e \bar{\rho}_s \bar{e}_v^{**}}{\bar{T}_e^2 \tau_{v-e}} + \frac{T'_e \bar{\rho}_s \bar{e}_v}{\bar{T}_e^2 \tau_{v-e}} - \frac{T'_e \bar{\rho}_s e_v^{*'}}{\bar{T}_e^2 \tau_{v-e}} + \frac{T'_e \bar{\rho}_s e'_v}{\bar{T}_e^2 \tau_{v-e}} - \frac{T'_e \rho'_s \bar{e}_v^{**}}{\bar{T}_e^2 \tau_{v-e}} + \frac{T'_e \rho'_s \bar{e}_v}{\bar{T}_e^2 \tau_{v-e}} - \frac{T'_e \rho'_s e_v^{*'}}{\bar{T}_e^2 \tau_{v-e}} + \frac{T'_e \rho'_s e'_v}{\bar{T}_e^2 \tau_{v-e}} \\
& + \frac{T'_v \bar{\rho}_s \bar{e}_v^{**}}{\bar{T}_v^2 \tau_{v-e}} - \frac{T'_v \bar{\rho}_s \bar{e}_v}{\bar{T}_v^2 \tau_{v-e}} + \frac{T'_v \bar{\rho}_s e_v^{*'}}{\bar{T}_v^2 \tau_{v-e}} - \frac{T'_v \bar{\rho}_s e'_v}{\bar{T}_v^2 \tau_{v-e}} + \frac{T'_v \rho'_s \bar{e}_v^{**}}{\bar{T}_{ev}^2 \tau_{v-e}} - \frac{T'_v \rho'_s \bar{e}_v}{\bar{T}_{ev}^2 \tau_{v-e}} + \frac{T'_v \rho'_s e_v^{*'}}{\bar{T}_{ev}^2 \tau_{v-e}} - \frac{T'_v \rho'_s e'_v}{\bar{T}_{ev}^2 \tau_{v-e}}
\end{aligned} \tag{B.9}$$

$$\begin{aligned}
\bar{\sigma}_{v-e} \approx & \frac{\bar{\rho}_s \bar{e}_v^{**}}{\bar{T}_e} - \frac{\bar{\rho}_s \bar{e}_v}{\bar{T}_e} + \frac{\bar{\rho}_s e_v^{*'}}{\bar{T}_e} - \frac{\bar{\rho}_s e'_v}{\bar{T}_e} - \frac{\bar{\rho}_s \bar{e}_v^{**}}{\bar{T}_v} + \frac{\bar{\rho}_s \bar{e}_v}{\bar{T}_v} - \frac{\bar{\rho}_s e_v^{*'}}{\bar{T}_v} + \frac{\bar{\rho}_s e'_v}{\bar{T}_v} \\
& - \frac{\bar{\rho}_s \bar{T}'_e \bar{e}_v^{*'}}{\bar{T}_e^2} + \frac{\bar{\rho}_s \bar{T}'_e e'_v}{\bar{T}_e^2} - \frac{\bar{T}'_e \bar{\rho}_s \bar{e}_v^{**}}{\bar{T}_e^2} + \frac{\bar{T}'_e \bar{\rho}_s \bar{e}_v}{\bar{T}_e^2} - \frac{\bar{T}'_e \bar{\rho}_s e_v^{*'}}{\bar{T}_e^2} + \frac{\bar{T}'_e \bar{\rho}_s e'_v}{\bar{T}_e^2} \\
& + \frac{\bar{\rho}_s e_v^{*'} \bar{T}'_v}{\bar{T}_v^2} - \frac{\bar{\rho}_s e'_v \bar{T}'_v}{\bar{T}_v^2} + \frac{\bar{T}'_v \bar{\rho}_s \bar{e}_v^{**}}{\bar{T}_{ev}^2} - \frac{\bar{T}'_v \bar{\rho}_s \bar{e}_v}{\bar{T}_{ev}^2} + \frac{\bar{T}'_v \bar{\rho}_s e_v^{*'}}{\bar{T}_{ev}^2} - \frac{\bar{T}'_v \bar{\rho}_s e'_v}{\bar{T}_{ev}^2}
\end{aligned} \tag{B.10}$$

B.5 Conduction

$$\sigma_{cond} = \frac{-1}{\bar{T}_k} \frac{\partial}{\partial x_j} \eta_k \frac{\partial \bar{T}_k}{\partial x_j} - \frac{1}{\bar{T}_k} \eta_k \frac{\partial T'_k}{\partial x_j} + \frac{T'_k}{\bar{T}_k^2} \frac{\partial}{\partial x_j} \eta_k \frac{\partial \bar{T}_k}{\partial x_j} + \frac{\partial}{\partial x_j} \eta_k \frac{T'_k}{\bar{T}_k^2} \frac{\partial T'}{\partial x_j} \tag{B.11}$$

where k is each of the energy storage mechanisms available to the molecule.

$$\bar{\sigma}_{cond} = \frac{-1}{\bar{T}_k} \frac{\partial}{\partial x_j} \eta_k \frac{\partial \bar{T}_k}{\partial x_j} + \frac{\bar{T}'_k}{\bar{T}_k^2} \frac{\partial}{\partial x_j} \eta_k \frac{\partial T'}{\partial x_j} \tag{B.12}$$

B.6 Molecular Depletion

$$\sigma_{dep} = \frac{\sum_{mol} \dot{w}_s \hat{D}_s}{\bar{T}} - \frac{\sum_{mol} \dot{w}_s \hat{D}_s}{\bar{T}_v} - \frac{T' \sum_{mol} \dot{w}_s \hat{D}_s}{\bar{T}^2} + \frac{T'_v \sum_{mol} \dot{w}_s \hat{D}_s}{\bar{T}_v^2} \quad (B.13)$$

$$\bar{\sigma}_{dep} = \frac{\sum_{mol} \dot{w}_s \hat{D}_s}{\bar{T}} - \frac{\sum_{mol} \dot{w}_s \hat{D}_s}{\bar{T}_v} \quad (B.14)$$

B.7 Electron Collisions

$$\begin{aligned} \sigma_{col} = -3 \sum_{heavy} (R_s \nu_{e,s}) [& 2\bar{\rho}_e - 2\bar{\rho}_e \frac{T'}{\bar{T}} - \bar{\rho}_e \frac{\bar{T}}{\bar{T}_e} + \bar{\rho}_e \frac{\bar{T}T'_e}{\bar{T}_e^2} - \\ & \frac{\bar{\rho}_e T'^2}{\bar{T}^2} + \bar{\rho}_e \frac{T'T'_e}{\bar{T}_e^2} - \bar{\rho}_e \frac{\bar{T}_e}{\bar{T}} + \bar{\rho}_e \frac{\bar{T}_e T'}{\bar{T}^2} - \bar{\rho}_e \frac{T_e'^2}{\bar{T}_e^2} - \bar{\rho}_e \frac{T'_e}{\bar{T}} + \bar{\rho}_e \frac{T'_e \bar{T}}{\bar{T}_e^2} + 2\bar{\rho}_e \frac{T'_e}{\bar{T}_e} - \bar{\rho}_e \frac{T_e'^2}{\bar{T}^2} \\ & 2\rho'_e - 2\rho'_e \frac{T'}{\bar{T}} - \rho'_e \frac{\bar{T}}{\bar{T}_e} + \rho'_e \frac{\bar{T}T'_e}{\bar{T}_e^2} - \rho'_e \frac{T'^2}{\bar{T}^2} + \rho'_e \frac{T'T'_e}{\bar{T}_e^2} - \rho'_e \frac{\bar{T}_e}{\bar{T}} + \\ & \rho'_e \frac{\bar{T}_e T'}{\bar{T}^2} - \rho'_e \frac{T_e'^2}{\bar{T}_e^2} - \rho'_e \frac{T'_e}{\bar{T}} + \rho'_e \frac{T'_e \bar{T}}{\bar{T}_e^2} + 2\rho'_e \frac{T'_e}{\bar{T}_e} - \rho'_e \frac{T_e'^2}{\bar{T}^2}] \end{aligned} \quad (B.15)$$

$$\begin{aligned} \bar{\sigma}_{col} = -3 \sum_{heavy} (R_s \nu_{e,s}) [& 2\bar{\rho}_e - \bar{\rho}_e \frac{\bar{T}}{\bar{T}_e} + \\ & \frac{\bar{\rho}_e \bar{T}^2}{\bar{T}^2} + \bar{\rho}_e \frac{\bar{T}T'_e}{\bar{T}_e^2} - \bar{\rho}_e \frac{\bar{T}_e}{\bar{T}} - \bar{\rho}_e \frac{\bar{T}_e'^2}{\bar{T}_e^2} - \bar{\rho}_e \frac{T_e'^2}{\bar{T}^2} \\ & -2\frac{\bar{T}'\rho'_e}{\bar{T}} + \frac{\bar{T}T'_e\rho'_e}{\bar{T}_e^2} - \frac{\rho'_e T'^2}{\bar{T}^2} + \frac{\rho'_e T'T'_e}{\bar{T}_e^2} + \\ & \frac{\bar{T}_e T' \rho'_e}{\bar{T}^2} - \frac{\rho'_e T_e'^2}{\bar{T}_e^2} - \frac{\rho'_e \bar{T}_e}{\bar{T}} + \frac{\rho'_e T'_e \bar{T}}{\bar{T}_e^2} + 2\frac{\rho'_e T'_e}{\bar{T}_e} - \frac{\rho'_e T_e'^2}{\bar{T}^2}] \end{aligned} \quad (B.16)$$

B.8 Impact Ionization

$$\sigma_{ion} = \frac{\sum_{ion} \dot{n}_{e,s} \hat{I}_s}{\bar{T}} - \frac{\sum_{ion} \dot{n}_{e,s} \hat{I}_s}{\bar{T}_v} - \frac{T' \sum_{ion} \dot{n}_{e,s} \hat{I}_s}{\bar{T}^2} + \frac{T'_v \sum_{ion} \dot{n}_{e,s} \hat{I}_s}{\bar{T}_v^2} \quad (\text{B.17})$$

$$\bar{\sigma}_{ion} = \frac{\sum_{ion} \dot{n}_{e,s} \hat{I}_s}{\bar{T}} - \frac{\sum_{ion} \dot{n}_{e,s} \hat{I}_s}{\bar{T}_v} \quad (\text{B.18})$$

Vita

Ethan Arthur Vogel was born September 27, 1995, in Greenville, South Carolina to Evan and Jean Vogel. He graduated from Wren High School in May, 2014 and then graduated from the University of Tennessee, Knoxville in May of 2018 with degree in aerospace engineering with a materials science and engineering minor. After that, he pursued his graduate degree in aerospace engineering with a concentration in thermal-fluid mechanics. His research interests are in scale-resolving simulations of high-speed flows and aerothermodynamics.