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Exploratory Studies of Turbulence/Chemistry Interaction in Hypersonic Flows

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Characterizing the effects of nonequilibrium chemistry on turbulence and the development of accurate prediction tools for hypersonic flows is essential for the design of future hypersonic flight technology. This paper is a summary of current exploratory studies of the interaction between turbulence and real gas effects using direct numerical simulation data of isotropic turbulence and turbulent boundary layers.

Introduction

The lack of understanding of turbulent hypersonic flows and the absence of accurate databases prevent the development of good turbulence models. The models that are used today in engineering production codes do not represent the effects of high compressibility and temperature levels in the turbulent regime. As a result, the chemical composition of the gas, the skin friction, and the heat transfer are not predicted accurately. Applications that are hampered by this lack of understanding include reusable launch vehicles, high-speed missile interceptors, hypersonic cruise vehicles, and reentry vehicles. With the increased interest in space exploration, the necessity for affordably accessing space to maintain telecommunication and space technologies, and the increased interest in atmospheric hypersonic flight, we need accurate techniques to predict and understand the flow phenomena in the turbulent flow regime over a wide range of conditions.

Let us consider some examples where the turbulence/real-gas effects are important. The external boundary layer on realistic hypersonic vehicles is simulated either assuming that the boundary layer is laminar or using simple turbulence models that have not been developed for hypersonic applications. In the flows of interest, the magnitude of the temperature fluctuations is significant due to the high energy content that is present. Furthermore, the chemical reactions are highly non-linear functions of the temperature. Therefore, turbulent temperature fluctuations result in large variations in the reaction rates. If we were able to perform accurate simulations of hypersonic flows, we would find a different chemical composition of the gas, and different reaction rates than those that are currently predicted.

DNS results of turbulent boundary layers[1] show that

under certain hypersonic flight conditions, a 5% temperature fluctuation results in a 30% fluctuation in the chemical composition of the gas. Thus, representing the chemical composition of the gas accurately is necessary to obtain accurate heating rates to the surface of hypersonic vehicles.

Real gas effects are also present inside a scramjet engine. Complicated shockwave patterns have been observed experimentally inside this type of engine (Calspan-University at Buffalo Research Center). Although these engines are being designed so that combustion occurs near the center of the engine and off the side walls, the high thermal loads resulting from shock impingement will lead to real gas effects near the walls. Thus, inside the engine the turbulent fluid motion is fully coupled to the chemically reacting processes. The turbulent mixing modifies the reacting mechanisms while the chemical heat release will induce compressions and expansions that may modify the internal flow field. Finally, the nonequilibrium expansion through the engine nozzle includes chemical recombination (heat release) and flow relaminarization. To accurately predict the propulsive thrust and aerothermal loads, turbulence models that accurately capture the shock/turbulence/real gas phenomena must be used.

Over the past decade, significant advances have been made in both experimental and computational research so that the "detailed" study of turbulence in the hypersonic regime can be accessed. In current work, we are building a DNS database of hypersonic flows.[2,3] Using reacting DNS data,[4-7] we have developed a preliminary understanding of the turbulence-chemistry interaction. A novel result obtained from this investigation is that depending on the hypersonic flight conditions, the chemical reactions damp or enhance the turbulent motion.[4,5] Figures 1 and 2 illustrate this result by showing the turbulence structures on boundary layers with different wall-temperature conditions and comparing the reacting and non-reacting (reactions are surgically turned off) results. For the
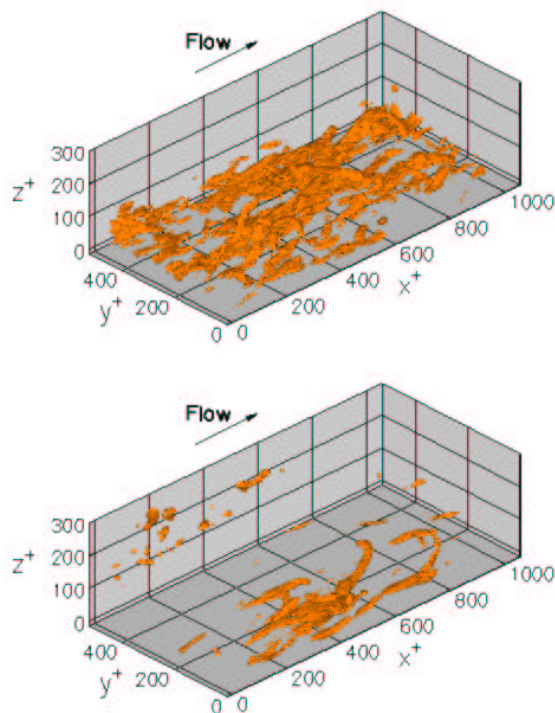
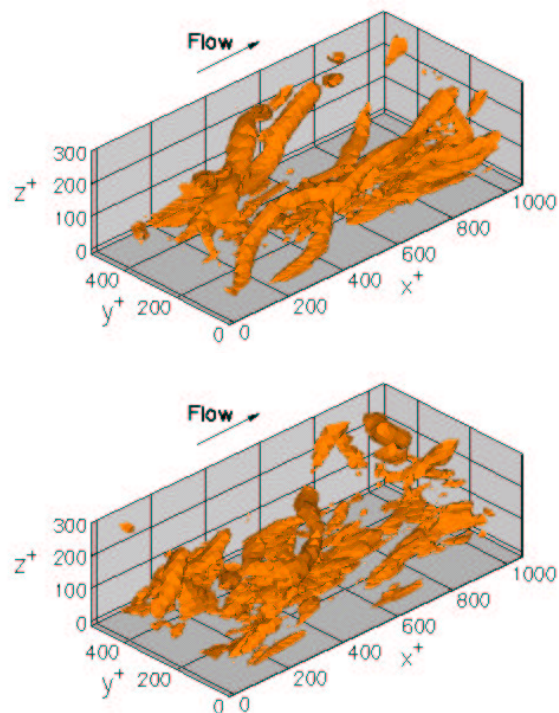**Fig. 1** Turbulence structures on the boundary layer over a 20° wedge flying at Mach 20, 20 km above sea level with adiabatic wall conditions. Top: No reactions; Bottom: Endothermic reactions. DNS data at $Re_\theta = 9480$.

Fig. 2 Turbulence structures on the boundary layer over a 20° wedge flying at Mach 20, 20 km above sea level with isothermal wall conditions. Top: No reactions; Bottom: Exothermic reactions. DNS data at $Re_\theta = 7225$.

case of an adiabatic wall temperature, Figure 1, chemical reactions are endothermic (energy is removed from the flow) across the boundary layer. We see that when the fluid is allowed to react the turbulence structures are nearly eliminated showing that the reactions damp the turbulent motion. In contrast, for an isothermal boundary layer, Fig. 2, the reactions are exothermic (energy is released) near the wall and the turbulence is enhanced. This can be observed by comparing the non-reacting and reacting results in Figure 2, where the structures for the reacting case are more chaotic. Such a result is relevant to the design of new air-breathing hypersonic vehicles since the drag and heat transfer would be reduced significantly when the reactions damp the turbulent motion. Thus by inducing endothermic reactions, cheaper and more efficient hypersonic vehicles could potentially be designed. On the other hand, if the flow conditions enhance the turbulence, accurate turbulence models must be developed to obtain accurate chemical composition and heating rates to the surface. A preliminary model for the closure of the chemical source term in turbulent hypersonic flows has been developed.[1, 8]

The preliminary turbulence model and the physical mechanisms behind it are not yet reliable as they must be studied under different flow configurations over a wide range of conditions. Moreover, experimental data is necessary to generalize the preliminary findings.

In this paper, the effect of turbulent fluctuations in the production of species is discussed. Exploratory studies of the turbulence/chemistry interaction and a preliminary scaling for the temperature fluctuation in terms of mean flow variables are presented. The assumptions that are used in the present study are also discussed. Conclusions and future work are then given.

The Chemical Source Term in Turbulent Flows

The chemical process is described by the production or destruction of species through the chemical source terms. There is also an energy exchange in the formation or destruction of molecular bonds. Thus, knowledge about the evolution of the chemical composition of the gas leads to an understanding of how much energy is exchanged due to chemical reactions. Therefore, modeling the turbulence/chemistry interaction mainly requires the accurate description of the chemical source terms.

For simplicity, let us consider the chemical source term $\overline{w}_s$ for a single nitrogen dissociation reaction, $N_2 + M \rightleftharpoons 2N + M$, assuming that the rotational and translational temperatures are in equilibrium and ne-

glecting the vibration and ionization processes. The consistency of these assumptions is described in a later section. The strong temperature-dependence of the source term can be seen by representing the variables as the sum of the mean and fluctuating values as $T = \overline{T} + T'$, for the temperature for example. The chemical source term, expressed as a first order approximation in fluctuations, is given by

$$
\begin{aligned}
w_{f\mathrm{N_2}} &= \overline{w}_{f\,\mathrm{N_2}} + \overline{w}_{f\,\mathrm{N_2}}\left(\left(\tfrac{\theta}{\overline{T}}+\eta\right)\tfrac{T'}{\overline{T}} + c'_{\mathrm{N_2}}\right) + \dots \\
w_{b\mathrm{N_2}} &= \overline{w}_{b\,\mathrm{N_2}} + \overline{w}_{b\,\mathrm{N_2}}\left(\left(\tfrac{\theta}{\overline{T}}+\eta\right)\tfrac{T'}{\overline{T}} - 2c'_{\mathrm{N_2}}\right) + \dots (1)
\end{aligned}
$$

where $\overline{w}_{f\,\mathrm{N_2}}$ and $\overline{w}_{b\,\mathrm{N_2}}$ are the forward and backward source terms for $\mathrm{N_2}$, and $w_s = w_{fs} + w_{bs}$, θ is the activation temperature, c_s is the mass fraction of species s, and $\overline{w}_f = w_f(\overline{T})$. We have also made use of the fact that $c'_{\mathrm{N}} = -c'_{\mathrm{N_2}}$, and we have assumed that the variation of K_{eq} in temperature is relatively weak, which is a good approximation at high temperatures. The variations of $w_{\mathrm{N_2}}$ caused by temperature fluctuations may be especially large because θ is typically an order of magnitude larger than the temperature. For air reactions, the fluctuations in the source term due to mass fraction variation are likely to be less important. Thus, to obtain accurate production of species we must model the temperature fluctuations.

In hypersonic flows, with the very high energies present and the highly non-linear relation between reaction-rate and temperature, the temperature fluctuations will be very large and in general:

$$
w_s(c_s, T) \neq w_s(\overline{c}_s, \overline{T}).
$$

A method for the closure of a non-linear term is the probability density function (PDF) approach,[9] in which the unclosed term is represented by a PDF in terms of the independent variables. Gaffney et al.[10] assume a PDF for the temperature fluctuations and investigate how the fluctuations affect the combustion process. Martin & Candler[8] follow a similar approach to account for the temperature fluctuation effect on $\overline{w}_s$. In particular, a PDF for the temperature fluctuations is calibrated using the DNS database[1,4,8] of canonical turbulent flows at typical hypersonic conditions. Therefore, the parameters that describe the PDF are based on resolved-scale turbulence data. This model represents the unresolved temperature fluctuations for use in Reynolds-Averaged Navier-Stokes (RANS) or large-eddy (LES) simulations of turbulence. During a RANS or LES calculation, we would construct the PDF that represents the temperature fluctuations based on the mean flow resolved parameters. Sampling from the PDF, we obtain the temperature fluctuation, which can then be combined with the mean temperature in the computation of the source term. The physical foundation of this preliminary model, its relevance and limitations are described later in the paper.
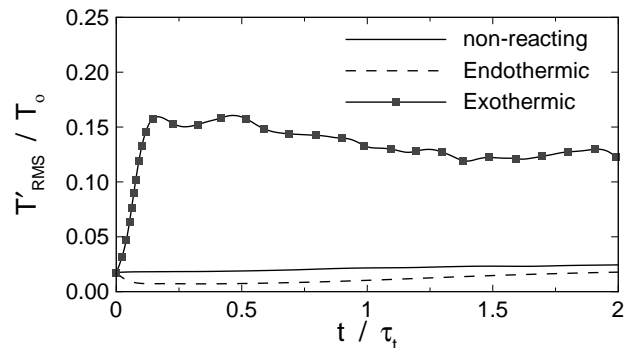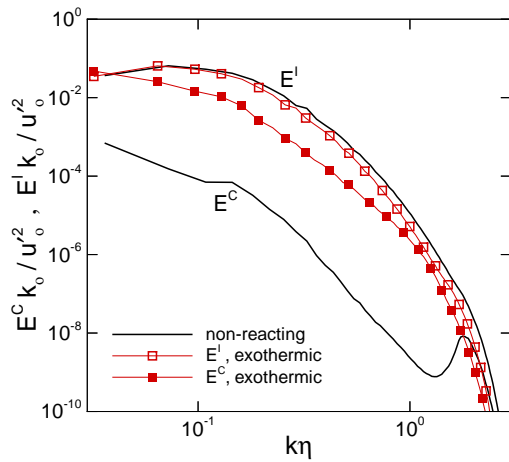

Fig. 3 Evolution of the temperature fluctuation magnitude in decaying isotropic turbulence for non-reacting, endothermic and exothermic simulations at conditions typical of hypersonic flows.

Turbulence/Chemistry Interaction

A parametric study of the turbulent/chemistry interaction for a single dissociation reaction in isotropic turbulence at conditions typical of hypersonic flows is conducted in Martin & Candler.[7] In this flow, the computational domain is a three-dimensional box, periodic in all directions. The mean velocity is zero, whereas the velocity fluctuations are non-zero. the turbulence decays in time as the chemical nonequilibrium reactions occur.

Figure 3 shows a typical result representing the effect of heat release on the normalized magnitude of the temperature fluctuations as the turbulence decays in time and the nonequilibrium reaction is progressed. The non-reacting case is shown for reference. For the endothermic case, the turbulent temperature fluctuations are damped. For the exothermic case, the temperature fluctuations are dramatically enhanced and nearly maintained during the turbulence decay.

The chemical reactions act as energy sources within the flow. Thus, a natural step is to study the energy dynamics. Figure 4 shows the energy spectra versus wave number comparing a non-reacting and an exothermic case. The wave number k represent the turbulent length scales; small k corresponds to large turbulent eddies and vice versa. The spectra have been decomposed into the compressible and incompressible energy modes,[11] E^C and E^I respectively. There is no significant effect of the heat release on the incompressible modes. In contrast, the energy in the compressible modes is significantly enhanced by the exothermicity of the gas. Also, we can see that the energy is equally placed among the turbulent length scales, showing that the chemical process is independent of length scale. This is because the reactions take place at the molecular level. Figure 5 shows the turbulent kinetic energy as a function of time for the non-reacting and exothermic cases. Whereas the viscous diffusion and viscous dissipation remain nearly unchanged, the
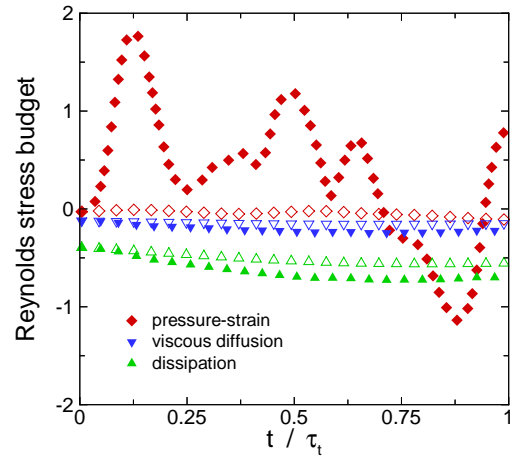
Fig. 4 Turbulent kinetic energy spectra in isotropic turbulence for non-reacting and exothermic simulations at conditions typical of hypersonic flows.

Fig. 5 Reynolds stress budget for the same simulations, empty symbols represent the non-reacting simulation.

Fig. 6 Turbulent kinetic energy profile in a Mach 4 turbulent boundary layer with isothermal wall-temperature conditions. Representative of the boundary layer on a $20°$ wedge flying at Mach 20, 20 km above sea level. DNS at $Re_\theta = 7225$.
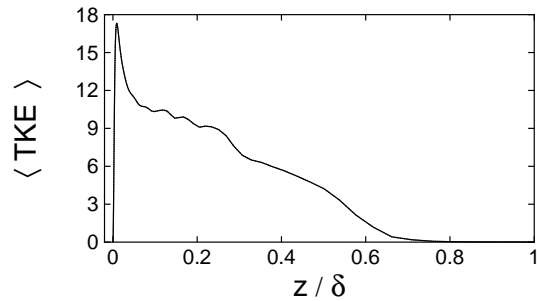
pressure-strain term is increased significantly by the exothermic reactions. This term has a characteristic oscillatory behavior and the non-dimensional period of oscillation is equal to the turbulent Mach number. This indicates that the oscillations are a result of acoustic waves. Thus, the generation of turbulent kinetic energy is mainly caused by compressibility effects which cause a feedback between the turbulence and the finite-rate reactions. The feedback is positive for exothermic reactions and negative for endothermic reactions.[7]

Reacting boundary layers are substantially more complex than isotropic turbulence. In a boundary layer, the mean temperature changes with distance from the wall. Typically, the maximum temperature occurs at some distance from the wall where there is significant shear-heating. At this location air molecules dissociate and the reaction products diffuse toward the wall, where they recombine due to the cool wall temperature. Therefore, in a boundary layer, there are endothermic and exothermic regions and how this regions interact in the presence of turbulence is difficult to diagnose.

In preliminary studies,[1] we performed DNS of adiabatic and isothermal boundary layers. In the adiabatic simulation, the temperature increases monotonically from the freestream to the wall. For the adiabatic conditions chosen, the temperature is always high enough to induce chemical reactions. Thus, the effect of endothermic reactions can be isolated. For the isothermal wall simulation, the near wall reactions are exothermic. The same results that were observed in isotropic turbulence are present in the boundary layer. Figure 6 shows the turbulent kinetic energy profile for the isothermal simulation, which is characterized by peaks and valleys. These peaks are not present in non-reacting boundary layers. This oscillatory behavior is also observed in the production and transport terms of both the turbulent kinetic energy budget and the evolution equation for the turbulent temperature fluctuation variance.[1] These preliminary results suggest that the peaks in the turbulent kinetic energy profile are a result of the positive feedback between the turbulence and the exothermic reactions.

Temperature Fluctuation Scaling

In preliminary results, we represent the temperature fluctuation distribution as a Gaussian PDF. The Gaussian distribution is described by a single parameter, the temperature fluctuation variance T'_{RMS}. Using the relation for the PDF variance and a conditional average, the temperature fluctuation variance can be

predicted. The DNS database shows that T'_{RMS} can be expressed as a function of the governing parameters.[4,8] For endothermic reactions, the temperature fluctuations scale linearly with the square of the turbulent Mach number, M_t^2. Whereas for exothermic reactions, the temperature fluctuations are enhanced and can be expressed as

$$T'_{RMS}/\langle T \rangle \quad = A(\overline{\Delta h^\circ}\ \lambda/l_E)^B \qquad (2)$$

where A and B are constants that depend on the specific reaction and $\overline{\Delta h^\circ}$ is the non-dimensional heat release. The variable λ, also known as the Taylor microscale, represents the distance traveled by a fluid particle moving at the speed of the turbulent intensity. The expansion length l_E is defined as the product of the speed of sound and the characteristic acoustic time scale, $a\,\tau_c$, which is the distance traveled by acoustic radiation from the chemistry-induced temperature fluctuations. Therefore, λ/l_E represents the ratio of the characteristic distance traveled by a typical particle of fluid to the characteristic distance traveled by the acoustic radiation. This scaling is consistent with the physical description of the interaction between finite-rate chemical reactions and turbulence that was given in the previous section.

Under the conditions chosen for the isotropic DNS data, λ/l_E was always less than one. As λ/l_E approaches one, $T'_{\mathrm{RMS}}/\langle T \rangle$ becomes large, indicating a strong turbulence/chemistry interaction. This occurs when the fluid travels a similar distance to the one covered by the acoustic radiation, which is induced by the temperature fluctuations. If λ/l_E were larger than one, the interaction would be expected to weaken because the turbulent motion would outrun the acoustic waves produced by the interaction, and the feedback process would be diminished. Also, as λ/l_E approaches zero the pressure waves outrun the fluid motion and the interaction is weak. Thus, the interaction weakens when λ/l_E departs from unity. In addition, $T'_{\mathrm{RMS}}/\langle T \rangle$ is affected by the heat released to the flow,[1] and the length ratio must be modulated by $\overline{\Delta h^\circ}$ to give an appropriate relation for the magnitude of the temperature fluctuations. When λ/l_E is greater than one, we would not expect this fit to be valid because it predicts a further strengthening of the interaction. The Reynolds number did not have a significant effect for the range of conditions that were considered. More details about the expression for T'_{RMS} can be found in Martin & Candler.[8]

All quantities on the right-hand side of Eq. 2 are known from the mean flow variables. Thus, this model is specially attractive since T' can be obtained from mean flow, resolved variables. Thus, the model can be implemented in the context of RANS or LES.

Figure 7 shows the normalized magnitude of the temperature fluctuations versus the heat ratio, $\overline{\Delta h^\circ}\lambda/l_E$, in isotropic turbulence using a single nitro-
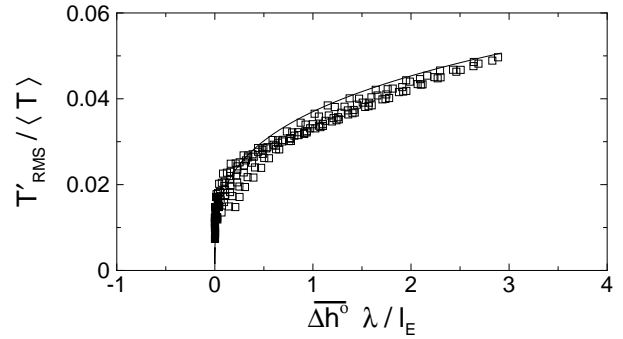
Fig. 7 Temperature fluctuation versus heat ratio in isotropic turbulence at conditions typical of hypersonic flows
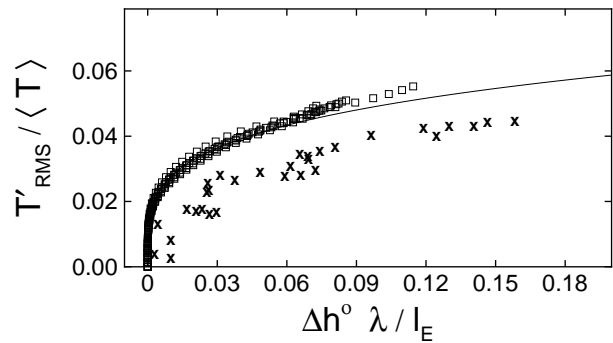
Fig. 8 Temperature fluctuation versus heat ratio in a Mach 4 turbulent boundary layer with isothermal wall-temperature conditions. Representative of the boundary layer on a 20° wedge flying at Mach 20, 20 km from the sea level. DNS at $Re_\theta = 7225$.

gen dissociation reaction where $N_2 + M \rightleftharpoons 2N + M$. The data include several simulations initialized at different chemical compositions of N_2 and N. Thus, the chemical nonequilibrium process evolves differently for each simulation as the turbulence decays. The data collapse using the relation in Eq. 2.

Figure 8 shows the normalized magnitude of the temperature fluctuations versus the heat ratio using the DNS database of a Mach 4 turbulent boundary layer with a single dissociation reaction using $S1 + M \rightleftharpoons S2 + M$, where S1 and S2 have the same number of internal degrees of freedom and the same molecular weight. This is a simplification so that changes in pressure are only due to changes in the density and temperature across the boundary layer. The reaction rates correspond to oxygen dissociation. The power law relation between temperature fluctuations and the heat ratio resembles that found in isotropic turbulence, and the data follow the same trend as that found in the isotropic turbulence. However, the data near the boundary layer edge do not collapse on the same curve. It is possible that this is because we have

not gathered sufficient statistics to get a large enough sample of data. A Reynolds number dependence is also possible. None of these reasons nor others can be proved true with the small dataset with which we are working. These results are preliminary, and we are performing further studies.

Assumptions of the Present Study

The previous studies are based on the following assumptions: (1) The translational and rotational temperatures are in equilibrium, and the vibration and ionization processes are neglected. (2) The reaction mechanism is represented by a single dissociation reaction as opposed to the mechanism of air. (3) For the boundary layer studies, the chemical composition of the gas is initialized at equilibrium based on the average temperature. In this section, we address the generality and limitations that are implied in these assumptions.

Assuming that the energy is characterized by a single temperature simplifies the turbulence/finite-rate-chemistry interaction and does not represent a limitation of the study. Let us consider the physical processes and conditions at which each of the temperatures (translational, rotational, vibrational and electronic) is in thermal-nonequilibrium with the other thermal modes and the possible effect of the temperature fluctuations.

It is well known that when a gas molecule travels through a shockwave the translational and rotational energy modes equilibrate within a few collisions, about 5 to 10. The reactions right behind a shockwave are endothermic as the gas dissociates due to the sudden increase in temperature. Thus, turbulent temperature fluctuations may not modify the reaction rates in the small nonequilibrium zone.

In contrast, the vibrational energy requires thousands of collisions to come to equilibrium with the other internal modes. Due to the high flow speed of the gas, there may exist a sizable nonequilibrium zone where the flow speed of the translational-rotational temperature and the vibrational temperature are different. We can observe the effect of the temperature fluctuations by linearizing the source term in the vibrational energy equation, which leads to a term similar to Eq. 1 but in terms of the activation energy for the vibrational modes, $\theta_v/\overline{T}$. The ratio of $\theta_v/\overline{T}$ is no larger than $\mathcal{O}(1)$ for typical hypersonic conditions. Thus, we may conclude that turbulent temperature fluctuations may affect the vibrational energy through the chemical source term w_s only. We are preforming studies to test this theory.

It is also assumed that there is no ionization. This assumption is valid depending on the chosen conditions. An estimate of the ionization fraction through a flow field can be found by calculating the equilibrium electron number density from the equilibrium constant for a particular reaction. This procedure severely over-estimates the actual ionization fraction because the electron producing reaction is much closer to being frozen than to being in equilibrium. We are considering conditions for which the ionization fraction is small so that no ionization is present.

Regarding the second assumption, for practical applications the temperature fluctuation model must be extended and calibrated to the air reaction mechanism. As a first step, we neglect the ionization of species, thus the reaction mechanism includes three collision induced dissociation reactions and two Zeldovich exchange reactions. The model must be generalized to this chemical mechanism and to include the effects of ionization and vibrational temperature.

The third assumption was made for two reasons. First, it allows us to isolate the effect of temperature fluctuations on the reaction rate. Second, we were unable to prescribe the correct chemical composition of the gas due to the lack of experimental data. Coupling experiments and computations, we will be able to relax the third assumption. The chemical composition of the gas could be prescribed by the experimental data. In turn, using the detailed experimental and computational database, we would be able to study and develop turbulence models for the interaction at realistic hypersonic conditions including thermo-chemical nonequilibrium.

Conclusions

A summary of the effect of finite-rate reactions on isotropic turbulence and turbulent boundary layers from direct numerical simulation data is provided. In these flows, the reaction rate varies exponentially with temperature, and thus small temperature fluctuations may cause large fluctuations in the rate of product formation. The direct numerical simulations show that there is a feedback between the chemical reactions and the turbulent motion. Endothermic reactions cause a reduction in the turbulence fluctuations and the feedback is negative. Whereas in the presence of exothermic reactions, the feedback is positive, and he turbulent fluctuations become more intense. The direct numerical simulation database reveals a physically consistent relation between the resolved-scale flow conditions that may be used to predict the turbulent temperature fluctuations, which in turn may be used to obtain accurate production of species. Further studies are necessary to generalize the findings that are summarized in this paper and to develop predicting tools for turbulent hypersonic flows.

Acknowledgments

References

[1] Martin, M. and Candler, G., "Temperature Fluctuation Scaling in Reacting Turbulent Boundary Layers," *AIAA Paper No. 01-2717*, 2001.

[2] Martin, M., "Preliminary DNS Database of Hypersonic Turbulent Boundary Layers," *AIAA Paper No. 03-3726*, 2003.

[3] Martin, M., Xu, S., and Wu, M., "DNS of Shock/Turbulent Boundary Layer Interaction," *AIAA Paper No. 03-3464*, 2003.

[4] Martin, M. and Candler, G., "Effect of Chemical Reactions on Decaying Isotropic Turbulence," *Physics of Fluids*, Vol. 10, 1998, pp. 1715–1724.

[5] Martin, M. and Candler, G., "DNS of a Mach 4 Boundary Layer with Chemical Reactions," *AIAA Paper No. 2000-0399*, 2000.

[6] Martin, M., "DNS and the LES Closure of Reacting Turbulence in Hypersonic Flows," *Ph.D. Thesis*, 1999.

[7] Martin, M., Olejniczak, D., Weirs, V., and Candler, G., "DNS of Reacting Hypersonic Turbulent Boundary Layers," *AIAA Paper No. 98-2817*, 1998.

[8] Martin, M. and Candler, G., "Subgrid-Scale Model for the Temperature Fluctuations in Reacting Hypersonic Turbulent Flows," *Physics of Fluids*, Vol. 11, 1999.

[9] Pope, S., "Methods for Turbulent Reactive Flows," *Prog. Energy and Combust. Sci.*, Vol. 11, 1985.

[10] Gaffney, R., White, J., and Drummond, J., "Modeling Turbulence/Chemistry Interactions Using Assumed PDF Methods," *AIAA Paper No. 92-3638*, 1992.

[11] Moyal, J., "The Spectra of Turbulence in a Compressible Fluid; Eddy Turbulence and Random Noise," *Proc. Cambridge Phil. Soc.*, Vol. 48, 1951, pp. 329.