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DSMC Study Of Flowfield And Kinetic Effects On Vibrational Excitations In Jet-Freestream Interactions

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Abstract. The Direct Simulation Monte Carlo (DSMC) computational technique was used to simulate the interaction between a carbon monoxide jet and a high velocity freestream of oxygen atoms oriented at 90° to the jet flow axis at 150km simulated altitude. The results of a study to characterize the sensitivity of predicted CO vibrational excitation to the vibrational excitation cross section and the nozzle exit plane profile are presented in this paper. A literature value of the vibrational excitation cross section is used as a baseline, and comparative simulations are made for cross sections that vary around that value. Similarly, the nozzle exit plane profile is varied from a "flat" profile to a fully developed laminar boundary layer profile to obtain sensitivities to the jet inflow startline. xSMILE, a software system based on the DSMC method, developed at the Institute of Theoretical and Applied Mechanics, Novosibirsk, Russia, has been utilized for this study. The results demonstrate a generally linear scaling of the vibrational excitation with cross section, except for cross sections that produce excitation rates in excess of the VHS gas kinetic rate. The jet exit-plane boundary layer profile was found to be a factor in the amount of CO excited state produced in the interaction region.

INTRODUCTION

Vibrational excitation of molecular species emitting from a jet into a high-speed, low density freestream is a process with importance to the prediction of high-altitude rocket exhaust plume infrared emissions. Accurate predictions of these emissions are necessary for the analysis of potential optical interference of on-vehicle instrumentation. Unfortunately, accurate vibrational excitation collision cross sections are not always available for the species pairs of interest and for the high relative energies encountered in this situation. In addition, nozzle exit plane flowfield characteristics are always a challenge to predict accurately. The purpose of this study is to test the sensitivity of predicted emissions to the excitation cross sections and nozzle exit plane flow parameters using the Direct Simulation Monte Carlo (DSMC) numerical technique.

Amine fueled thrusters can contain significant mole fractions of CO in their exhaust flow. At altitudes above 100km, oxygen atoms make up a large fraction of the atmosphere. Significantly, the O + CO vibrational excitation cross section is very high compared to the excitation cross sections for other atmospheric gases, and can produce excitation of CO vibrational states, leading to IR emission, when the atmosphere encounters a thruster exhaust plume at high relative velocities. This is the system that we chose to analyze for this study.

SIMULATION CONFIGURATION

For simplicity, we used an exhaust flow of pure CO expanding into a low density atmosphere of oxygen atoms. The configuration is illustrated in Figure 1. A high-speed freestream of oxygen atoms encounters a jet of CO expanding from the "sidejet" of a rocket such that the freestream flow velocity vector and jet centerline are at 90°. The flow parameters for both the jet and freestream are also shown in Figure 1. The oxygen atom density corresponds to that found at an altitude of 150km, assuming an oxygen atom mole fraction of 0.33 at that altitude.

The sidejet exit plane is 0.15 m in diameter and is placed a distance of 1.5 m behind the nose of the rocket, which is 0.5 m in diameter.

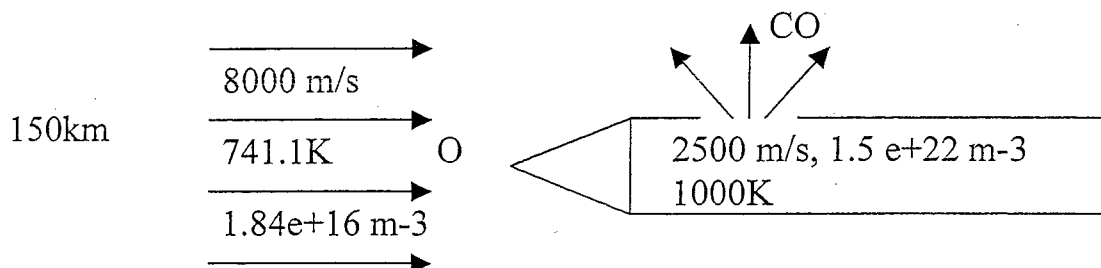


FIGURE 1. Simulation Configuration Showing Jet and Atmosphere Flow Parameters.

NUMERICAL METHOD

The SMILE three-dimensional DSMC code system¹ developed at the Institute of Theoretical and Applied Mechanics was used in this study. This package includes a GUI interface to access the DSMC solver. SMILE uses the variable hard sphere model² for gas-gas collisions and the total collisional energy model² for chemical reactions. A species weighting scheme³ is also implemented to allow increased statistical accuracy for minor gas species in the flow.

The gas density at the sidejet exit plane is relatively high and the corresponding Knudsen number is low, making a full DSMC calculation including the near exit plane region along with the far field regions difficult. Consequently, a convenient feature of the SMILE package is utilized. An axisymmetric simulation of the near exit plane jet expansion flow region is first carried out, with no freestream flow. A three dimensional startline taken at a position away from the high density region is then determined from this calculation and used for the subsequent full flowfield calculation. This two-step process assumes that the freestream does not affect the jet expansion flow in the jet near field. The results show that this assumption is correct for this high altitude case.

Although vibrational excitation and relaxation is usually handled in DSMC by the Borgnakke-Larson method, with either a fixed or temperature-dependent probability of excitation per collision, we model the vibrational-translation (V-T) exchange process as a chemical reaction: $\text{CO} + \text{O} \rightarrow \text{CO}^* + \text{O}$, where CO^* is the vibrationally excited state of CO. The reverse (quenching) reaction is also modeled. These are the only reactions allowed in the simulation. This approach allows for a more precise specification of the cross section as a function of energy and a more direct comparison with existing experimental and theoretical results. It is assumed that any molecular dissociation or recombination reactions will be negligible at this velocity and so would have little impact on the CO + O vibrational excitation process.

The vibrational excitation of CO by O at 8000 m/sec has been measured by Upschulte and Caledonia.⁴ In their crossed beam experiment, they noted a highly excited vibrational state distribution, but did not have the spectral resolution to allow a determination of the excitation cross section for individual CO vibrational states. Their cross section of $7.3 \times 10^{-21} \text{ m}^2$ for the "average cross section for one quantum of vibrational excitation" is used here as the CO^* excitation cross section. In our simulation there is no specificity as to the exact vibrational state distribution produced. Any analysis requiring specific information on the excited state population in the flow would by necessity require the vibrational excitation cross sections for each vibrational state, as well as modeling of vibrational-vibrational (V-V) and state specific V-T collisional exchange. We also do not model radiative decay out of CO^* .

In the DSMC chemistry model, reaction cross sections and, more specifically, reaction probabilities, are internally determined from the user specified Arrhenius parameters, A, n, and E_a , used to define the reaction rate:

$$k_r = AT^n e^{-E_a/RT}$$

where A and n are constants and E_a is the activation energy. Here we assume $n=0$, and $E_a = 4.252 \times 10^{-20} \text{ J}$ (3.4 eV), the energy of the $v=1$ level of CO. Backing out a value of A from the experimentally determined cross section yields $A = 6.455 \times 10^{-17} \text{ m}^3/\text{s}$.

RESULTS AND DISCUSSION

The baseline case uses a jet exit plane laminar boundary layer profile based on a conical nozzle calculation using a 15° half angle expansion to an area ratio of 10. The exit plane was then split into 5 radial sections, reduced in size moving from the centerline to the wall to capture the relatively thin boundary layer, and the corresponding flow parameters in each section were determined for use in SMILE as the jet inflow boundary. The number density was adjusted to match the total flux from a jet with a flat exit plane density and velocity profile (the values given in Figure 1).

A contour plot of the CO^* number density for the baseline case along the $Z=0$ plane (centerline of the rocket) is shown in Figure 2. The origin in this and all of the following figures is at the rocket nose, with the center of the axisymmetric sidejet at $x=1.5\text{m}$. It is apparent that, for these conditions, significant CO^* is produced by excitation of CO in the jet by the freestream O. Similar views for the CO and O number densities are shown in Figures 3 and 4. It is apparent that the high speed freestream does little to disturb the radially expanding CO jet. O atoms in the freestream show no shock buildup upon encountering the jet, but do show a significant depletion as they move through the jet expansion. Simulations with quenching collisions suppressed were carried out and there was no quantitative difference in the results, showing that this CO^* depletion mechanism does not occur for this low density case.

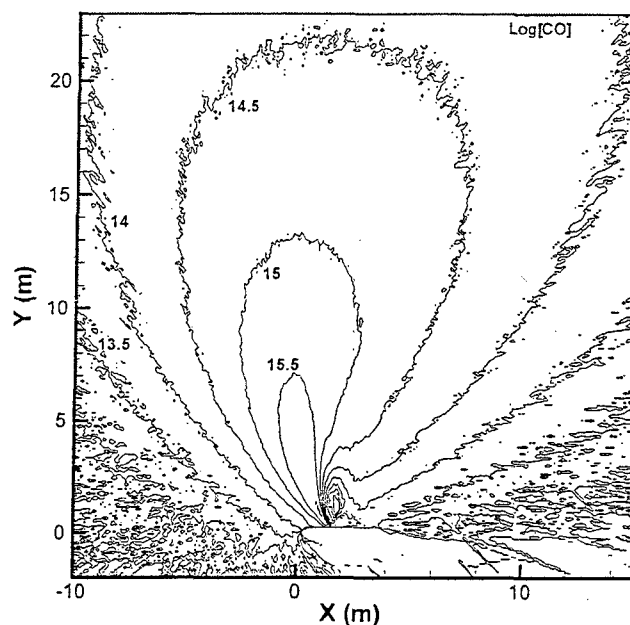


FIGURE 2. $[\text{CO}^*]$ along $Z=0$ symmetry plane.

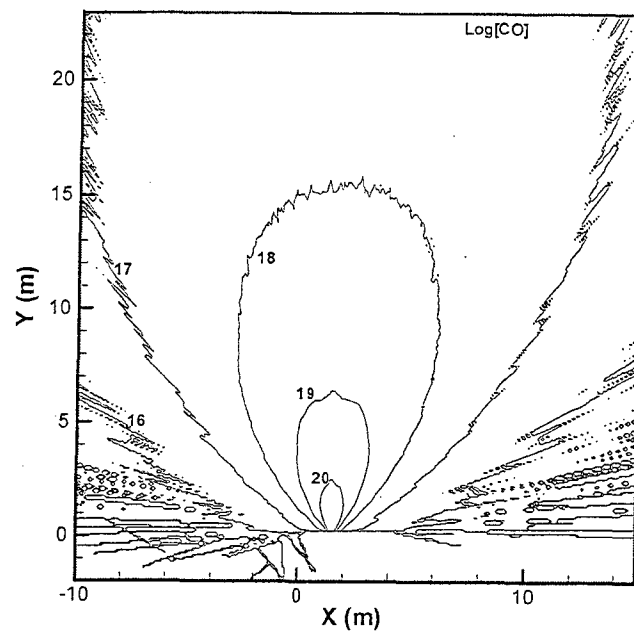


FIGURE 3. $[\text{CO}]$ along $Z=0$ symmetry plane.

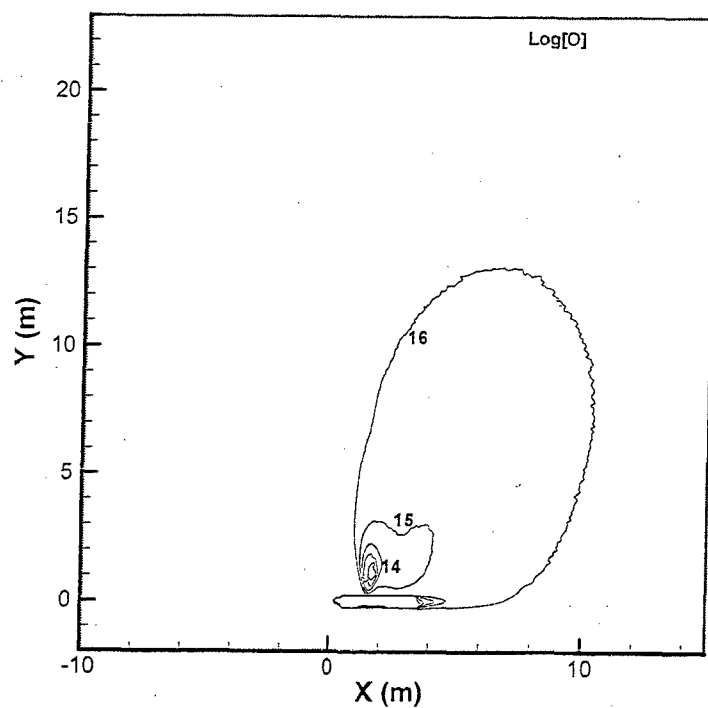


FIGURE 4. $[\text{O}]$ along $Z=0$ symmetry plane.

Effects of Collision Cross Section

Reliable values for reaction rates or collision cross sections are notoriously difficult to obtain at high energies, so a significant uncertainty in the parameters used is always present in this type of simulation. For the particular process examined here, a quasi-classical trajectory (QCT) study has been performed by Braunstein and Duff,⁵ which predicts a cross section at 8000 m/s for excitation into all vibrational levels that is about one order of magnitude higher than the value reported by Upschulte and Caledonia.⁴ Braunstein and Duff discuss the possibility that the experimental results were not fully in the single-collision regime, which would make their reported cross section a lower-bound value. To examine the effect of the uncertainty in the reaction parameter values, three additional cases were run using cross sections (A values) 10, 100, and 1/100 of the baseline cross section. To illustrate the differences in the results, the CO* number density along a cut at Y=4m is shown in Figure 5. In addition, the total CO* produced in the calculational domain for each case is shown in Table 1.

As seen in Figure 5 and Table 1, if the value of A is decreased by 100X, or increased by 10X, then the amount of CO* produced decreases or increases by approximately the same factor. However, if the value of A is increased by 100X, the amount of CO* produced increases by only about 20X. This can be understood by the cross sections shown in Figure 6, and by recalling that collision processes in DSMC are actually handled in terms of probabilities. The cross section for the reaction considered here using the baseline parameters and the total collision energy model is displayed, using equation 6.8 from ref. 2 and assuming that $\zeta=0$. (In actuality, the SMILE code uses $\zeta=1$, which will shift the resulting computed cross section in the region where the collision energy is close to E_a , but at the energies we are considering the effect is smaller than 30%. This is shown in fig 3 of Braunstein and Wysong.⁶) We note that the cross section is fairly flat at energies greater than twice E_a . This is due to the assumption that $n=0$. For non-zero values of n , the cross section would either increase or decrease significantly at higher energies.

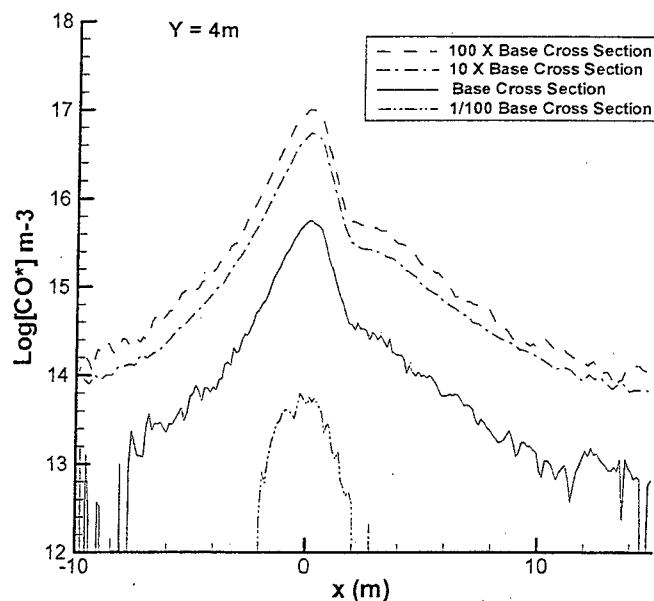


FIGURE 5. Collisional excitation cross section effects on CO* number density at Y=4m.

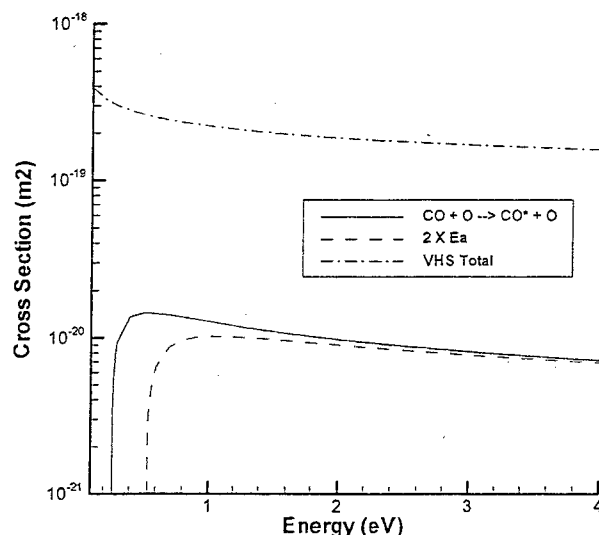


FIGURE 6. Cross Section Comparison.

At the collision velocity of 8000 m/s, the energy is 3.4 eV and the excitation cross section is $8 \times 10^{-21} \text{ m}^2$. The VHS total collision cross section as a function of collision energy is also shown in Figure 6 (using $d_{\text{ref}} = 3.725 \times 10^{-10} \text{ m}$, $\omega = 0.75$, $T_{\text{ref}} = 273 \text{ K}$), and the value at 3.4 eV is $1.6 \times 10^{-19} \text{ m}^2$. The ratio gives a probability per collision of 0.05. If the value of A were increased by a factor of 20, the probability per collision would be unity. Any further increase in the value of A will have a very small effect on the reactions in the simulation, since every O-CO collision at the most probable collision energy is already producing a CO^* . It has been discussed previously⁷ that use of parameters that produce reaction probabilities greater than unity will produce a systematic bias in results; the present study shows an example for an actual flowfield. A related point is that the use of a higher value of n (n=2, for example) could produce a reasonable agreement with measured reaction rates at low energies but would predict a reaction probability greater than unity for the energy considered here.

For chemical reactions and vibrational excitation/relaxation, it is not expected that the true cross section will ever exceed the gas kinetic (roughly equivalent to the VHS total) cross section. However, certain cases of rotational relaxation are known to be extremely fast, and measurements of the total rotational relaxation cross section for NH_3 , for example, exceed the gas kinetic cross section.⁸

TABLE 1. Total Domain CO^*

Cross Section Multiplier	Total CO^*
0.01	6.47×10^{14}
1	6.29×10^{16}
10	6.31×10^{17}
100	1.14×10^{18}

Effects of Activation Energy

The value of the E_a parameter also has significant uncertainty. The value assumed here is equal to the energy spacing between the ground and first excited vibrational level and represents a lower bound to E_a . However, the impulsive nature of collisions that produce vibrational excitation tends to lead to an effective value of E_a that exceeds the energy of the excited level. Measurements of the rate coefficient as a function of temperature and QCT calculations of the cross section⁵ both indicate that the value of E_a should be closer to 0.46 eV. A different value of

E_a , as seen in Figure 6, changes the resulting reaction cross section by orders of magnitude for collisions that have energies close to E_a , but has a small effect on collisions with energies that are much higher, since the cross section becomes very flat at higher energies. (As discussed above, this is similar to the effect of changing the assumed value of ζ .)

Figure 7 shows the effect on CO^* production of increasing the baseline value of E_a by a factor of 2. The resulting peak value of CO^* is decreased by less than 30%. However, it is somewhat surprising that any effect is seen, since the low density of O in this flowfield results in nearly single-collision conditions for O-CO at an energy of 3.4 eV. The visible effect may be due to the fact that collisions are not monoenergetic but reflect sampling based on the respective gas temperatures, as well as a small contribution from secondary collisions. Any secondary collisions will have lower energies and will be more sensitive to the differences in reaction parameters.

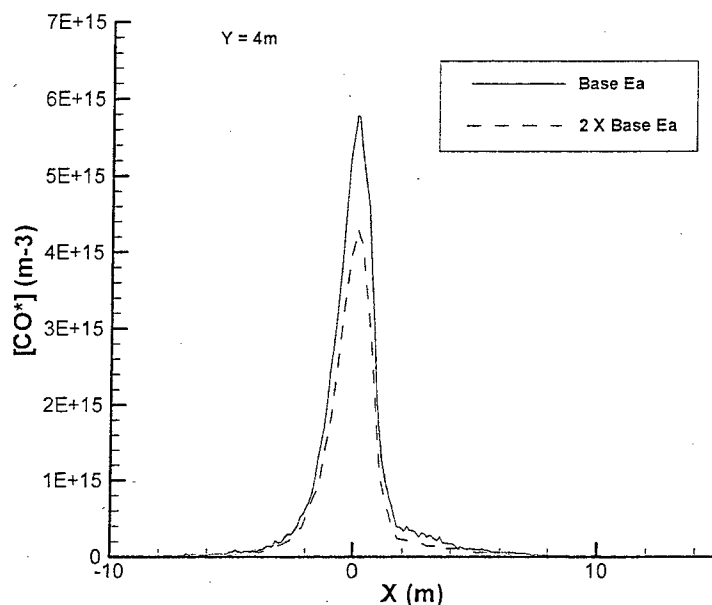


FIGURE 7. Effects of activation energy on CO^* number density at $y=4\text{m}$.

Effects of Jet Exit Plane Profile

The boundary layer profile at the jet exit plane can have a significant impact on the expansion flow structure, particularly at high off axis angles. The flow in this "backflow" region originates in the boundary layer near the nozzle wall where the flow parameters deviate the most from the center core of the expansion. Recently, a similar DSMC sidejet study⁹ showed significant jet exit plane profile effects on the flow structure, on the species produced by chemical reactions in the flow, and on the flux to the rocket body surface for a 5 km/s atmosphere at 120 km impinging on a simulated amine thruster exhaust flow. Here we compare the impact of the boundary layer structure by simulating a jet exit plane flow with a flat profile and comparing the results with the baseline case of a developed boundary layer. The CO number density and longitudinal velocity profile at the jet exit plane are shown in Figure 8. Here we see the result of adjusting the number density of the gradient profile to match the total flux of the flat profile. Because the velocity near the wall for the gradient profile is much lower than that at the centerline of the flow, the number density in the center portion of the expansion is significantly higher than for the flat profile, but the number density near the wall is still considerably lower.

The CO^* number density along a 4m cut is shown in Figures 9 and 10. On a log scale (Figure 9) it is apparent that, for the case with a boundary layer, more CO from the jet expands into the very high angle region, and therefore generates more CO^* in that region. On a linear scale (Figure 10) it is seen that the flat profile produces more CO^* in the region where most of the CO^* is produced. This region of highest CO^* production is at significant angles from the jet flow axis ($>30^\circ$ – see Figure 2 – recalling that the jet center is at $x=1.5\text{ m}$), and consequently, the flow

originates from the portion of the jet exit plane where the CO density for the flat profile is actually higher than that for the gradient profile, and thus produces the higher level of CO*. For this cut, the peak is about 30% higher for the flat profile.

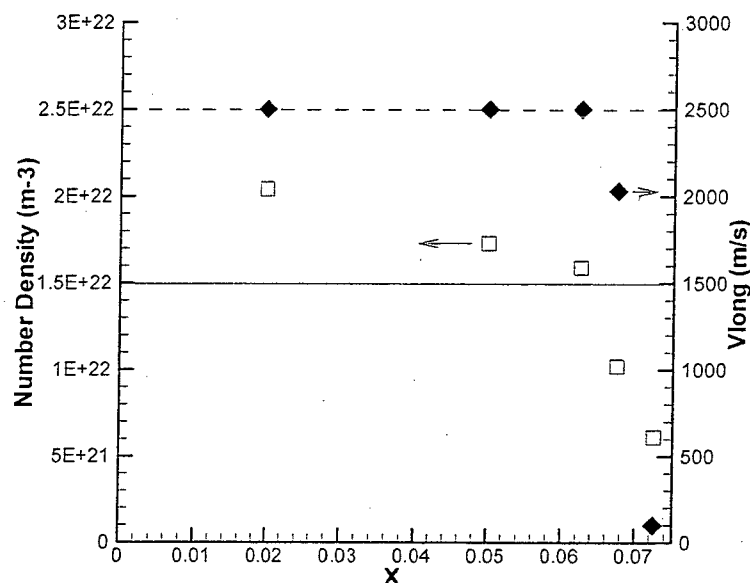


FIGURE 8. Number Density and Longitudinal Velocity Profiles at Jet Exit Plane. Dotted line is the velocity for a flat profile, solid line is the number density for a flat profile.

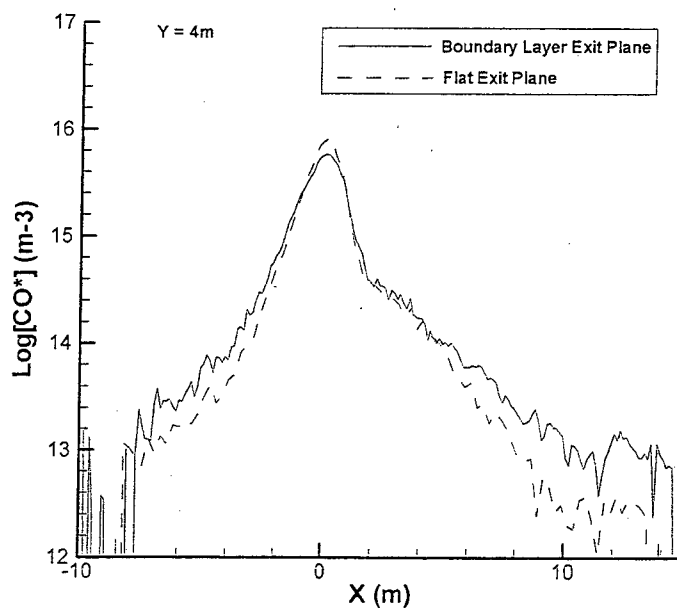


FIGURE 9. Effects of Boundary Layer on CO* at $Y=4$ m. Log Scale.

We conclude from these results that the exit plane profile can affect the production of collisionally excited molecules in the flow, but if the total amount of excitation produced in the flow is of concern, the difference is not large. If, on the other hand, the amount of produced excited states directly in front of the vehicle is of concern, then the effects of the jet exit boundary layer structure can be large, as illustrated in Figure 11, which shows a profile of the CO^* number density along a $Y=1\text{m}$ cut. At any given point along this profile, the gradient exit plane profile is a factor of 2 and more greater than that produced by the flat profile, with the difference being larger closer to the vehicle nose.

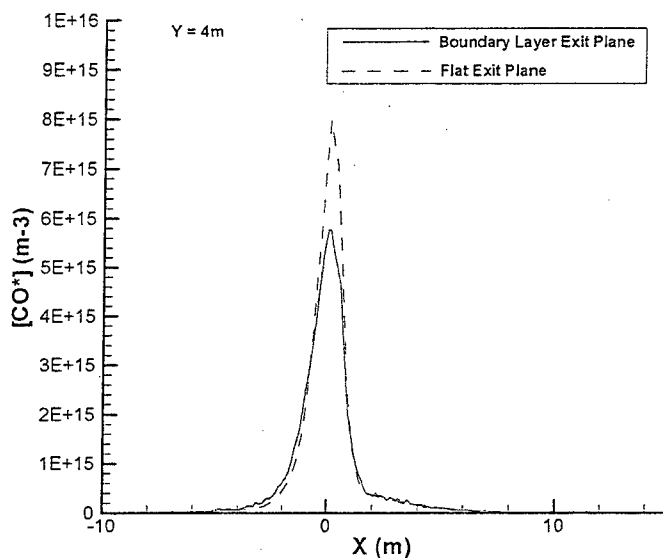


FIGURE 10. Effects of Boundary Layer on CO^* at $Y=4\text{m}$. Linear Scale.

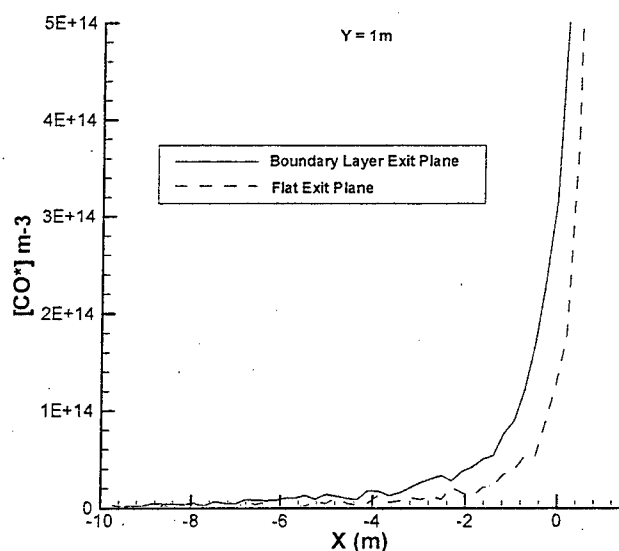


FIGURE 10. Effects of Boundary Layer on CO^* at $Y = 1\text{m}$.

SUMMARY AND CONCLUSIONS

The effects that we have seen on the production of CO* in a jet of CO expanding into a high speed freestream of O atoms have demonstrated that linear scaling with vibrational excitation cross section occurs for excitation rates below gas kinetic. Above gas kinetic rates, the assumptions inherent in the VHS collisional model prevent the excitation from continuing to increase. In addition, some sensitivity to the activation energy in the Arrhenius chemistry model was observed even in this high energy case where the collisional energy is far from threshold. Finally, the boundary layer structure at the jet exit plane has been found to affect the amount of excitation in the flow, with the magnitude of that effect dependent on the region of the flow that is of concern.

It should be pointed out that the quantitative effects of kinetic processes and jet exit plane flow structure on the production of excited states in a molecule of interest will depend on the altitude (freestream density), the relative jet-freestream velocity, and the species pairs of interest. The results of this study for one set of flow parameters should not be extrapolated to other cases. This is especially true for lower altitudes (higher freestream densities) and lower freestream velocities, where significant density shocks will occur in the flow and where the collisions are closer to excitation threshold energies. Multiple collisional effects at lower altitudes likely will have a large impact on the excitation/quenching processes. Simulations for specific conditions will be necessary to accurately characterize each situation.

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