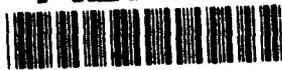


AD-A276 692



2

PL-TR-93-2177

SIMULATION OF CO₂ RELEASE AT 800 KM ALTITUDE

A. Setayesh

Radex Inc.
Three Preston Court
Bedford, MA 01730

DTIC
SELECTE
FEB 24 1994
S B D

August 31, 1993

Scientific Report No. 7

22 PD 94-06032

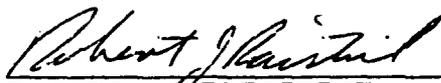
Approved for public release; distribution unlimited



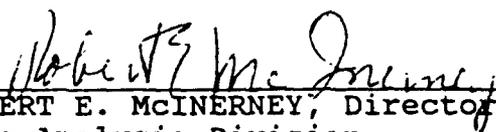
PHILLIPS LABORATORY
Directorate of Geophysics
AIR FORCE MATERIEL COMMAND
HANSCOM AIR FORCE BASE, MA 01731-3010

94 2 28 268

"This technical report has been reviewed and is approved for publication"



ROBERT J. RAISTRICK
Contract Manager
Data Analysis Division



ROBERT E. MCINERNEY, Director
Data Analysis Division

This report has been reviewed by the ESD Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS).

Qualified requestors may obtain additional copies from the Defense Technical Information Center. All others should apply to the National Technical Information Service.

If your address has changed, or if you wish to be removed from the mailing list, or if the addressee is no longer employed by your organization, please notify GL/IMA, Hanscom AFB, MA 01731. This will assist us in maintaining a current mailing list.

Do not return copies of this report unless contractual obligations or notices on a specific document requires that it be returned.

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE 31 August 1993	3. REPORT TYPE AND DATES COVERED Scientific Report No. 7		
4. TITLE AND SUBTITLE Simulation of CO ₂ Release at 800 km Altitude		5. FUNDING NUMBERS PE 63220C PR S321 TA 85 WU AC Contract F19628-90-C-0191		
6. AUTHOR(S) A. Setayesh				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) RADEX, Inc. Three Preston Court Bedford, MA 01730		8. PERFORMING ORGANIZATION REPORT NUMBER RXR-93081		
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Phillips Laboratory 29 Randolph Road Hanscom AFB, MA 01731-3010 Contract Manager: Robert Raistrick/GPD		10. SPONSORING / MONITORING AGENCY REPORT NUMBER PL-TR-93-2177		
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for Public Release Distribution Unlimited		12b. DISTRIBUTION CODE		
13. ABSTRACT (Maximum 200 words) The SOCRATES contamination-interaction code has been used to simulate the reactions of O + CO ₂ - CO ₂ (v) + O, O + CO ₂ - CO(v) + O ₂ , and CO ₂ + H - CO + OH(v) at an altitude of 800 km in both ram and wake directions of the spacecraft. These simulations show that the radiation from these reactions can be measurable for the parameters which have been used in these calculations. The investigation carries out the simulations as much as 30 km from the spacecraft. The radiative intensity of CO(v) and OH(v) show the highest and lowest, respectively.				
14. SUBJECT TERMS Gas plume, CO ₂ , CO, and OH emissions, Monte Carlo method, rarefied flows		15. NUMBER OF PAGES 22		16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT Unlimited	

TABLE OF CONTENTS

<u>Section</u>	<u>Page</u>
1. INTRODUCTION	1
2. DESCRIPTION OF THE MODEL CONFIGURATION	2
3. DESCRIPTION OF THE SOCRATES CODE	2
4. DISCUSSION OF RESULTS	4
5. SUMMARY AND CONCLUSIONS	16
6. REFERENCES	17

Accession For	
DTIC GRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By _____	
Distribution/_____	
Availability Codes	
Dist	Avail and/or Special
A-1	

LIST OF FIGURES

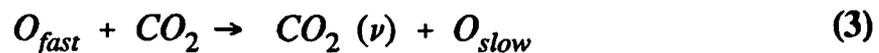
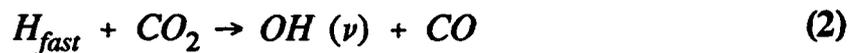
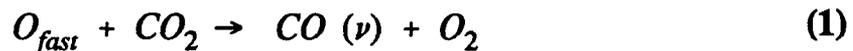
<u>Figure</u>	<u>Page</u>
1. Contour plots showing the CO ₂ vibrational excitations at 4.3 μm	5
2. Contour plots showing the CO vibrational excitations at 4.7 μm	6
3. Contour plots showing the OH vibrational excitations at 2.7 μm	7
4. Contour plots showing the CO ₂ , CO, and OH vibrational excitations for the same scale	8
5. Contour plots showing the CO ₂ reaction rates	9
6. Contour plots showing the CO reaction rates	10
7. Contour plots showing the OH reaction rates	11
8. Contour plots showing the CO ₂ , CO, and OH reaction rates for the same scale	12
9. Gray scale plots showing the intensity of CO ₂ at the time of release .	13

LIST OF TABLES

<u>Table</u>	<u>Page</u>
1. Molecular Parameters Used in the Calculations	4
2. Rate Coefficient Used in SOCRATES	14
3. Parameters Used in the Simulations	14

1. INTRODUCTION

The present work is based on simulation of CO₂ released at an altitude of 800 km in both the ram and wake directions of the spacecraft using the SOCRATES (Spacecraft/Orbiter Contamination Representation Accounting for Transiently Emitted Species) code. SOCRATES is a Monte Carlo code which calculates scattering, collisional excitations, and reactive collisions [Elgin, *et al.*, 1990]. The code will be discussed in more detail later. The primary purpose of the simulation is to study the collisional excitation of CO₂ with atmospheric oxygen and hydrogen atoms. The reactions of CO₂ with oxygen can produce the vibrational excitation of CO₂ and CO. Similarly, the CO₂ reaction with hydrogen atoms produce vibrationally-excited OH. This parametric study is a continuation of earlier work on the subject [Setayesh, 1991]. The current investigation carries out the simulations in two directions to a distance of as much as 30 km from the point of origin. The reactions of CO₂ with atomic oxygen and hydrogen are:



Reaction (4) represents the collisional transfer of kinetic energy to vibrational energy. Reactions (5) and (6) are reactive collisions which do not proceed at room temperature due to large activation energies [Elgin, *et al.*, 1990].

2. DESCRIPTION OF THE MODEL CONFIGURATION

The model configuration is based on a proposed gas release experiment on the ARGOS satellite. The satellite is expected to be in a circular orbit at an altitude of approximately 800 km with an orbital velocity of 7.4 km/s. The CO₂ release experiment will be one of many experiments to be conducted onboard the satellite [Lai, *et al.*, 1992]. A nozzle with a small diameter is assumed to be the source of the CO₂ gas released into space from a space platform. The diameter of the nozzle and mass flow rate of the CO₂ remain constant. Two conditions for the release will be considered here: one in the ram direction, and the other in the wake direction. It is also assumed that the gas release will last approximately 1.0 second (from a fraction of a second to several seconds has been proposed in the actual experiment). The temperature of the CO₂ gas at the time of the release is assumed to be about 50° C. The solution domain in the steady state (for both reactions) is taken to be a cubic space of 28,800 km³ in volume (32 by 30 by 30 km³) consisting of 8400 unevenly spaced cells. In each cell, there are 3 to 20 molecules (depending upon the density of species and cell location) for each species.

3. DESCRIPTION OF THE SOCRATES CODE

The SOCRATES contamination-interaction code has been developed to model contamination on spacecraft and to study the neighboring flow field around the shuttle [Elgin and Sundberg, 1988]. In the SOCRATES code, the direct simulation Monte Carlo technique has been revised and extended significantly to account for the energy dependent collision cross sections [Bird, 1981] and a statistical collision model for internal energy effects [Borgnakke and Larsen, 1975] which have been described by Elgin and Sundberg [1988] and Elgin, *et al.*, [1990]. In the code, the collision cross section is defined by the variable hard sphere model (VHS) which is a function of the relative velocity between two molecules. The collision cross section can be stated as

$$\sigma = \sigma_{ref} \left(\frac{v_r}{v_{ref}} \right)^{-2\omega} \quad (4)$$

where σ_{ref} and v_{ref} are the reference collision cross section and velocity, respectively [Elgin, *et al.*, 1990]. ω is a constant parameter which has a value of 0.25 for this investigation.

Reactive collisions between molecules and/or atoms (which are relevant to the present work) can be simulated directly by SOCRATES. The reaction cross section is a function of the relative collision energy as defined by Equation (4). The Monte Carlo program, in the event of collision, simulates the reaction with a probability which is related to the ratio of the reactive cross section to collision cross section at the relative velocity for the collision [Elgin and Sundberg, 1988].

The present work employs the option of using the Arrhenius rate constant in the code to calculate the rate of reactive collisions. The rate constant has the form of

$$k_r = A T^n e^{-\frac{E_a}{R_0 T}} \quad (5)$$

where A and n are constant parameters, R_0 and T are gas constant and temperature, respectively, and E_a is the activation energy. In the case of the collision between two reactants, the reaction cross section is calculated, and the reaction is counted with a weighing factor W_r . The weighing factor is given by

$$W_r = W_c \frac{v_r \sigma^*}{v_r \sigma} \quad (6)$$

where σ^* , σ , and W_c are the reactive cross section, collision cross section, and collision weighing factor, respectively. Further discussion of the reactive collisions can be found in the report by *Elgin and Sundberg* [1988].

4. DISCUSSION OF RESULTS

The simulation for the reaction of CO₂ with O and H for the altitude of 800 km are presented in panels of tables and plots for two cases of ram and wake directions. Tables 1-3 represent the parameters used for the simulation. Figures 1-3 and 5-7 show panels of contour plots of radiation intensity and reaction rates for CO₂, CO, and OH, respectively, in the ram and wake directions. Figures 4 and 8 show the combination of cases presented in Figures 1-3 and 5-7, respectively. Figure 9 shows the gray plot for CO₂ density distribution in the ram and wake directions. The asterisks in the figures and the text denote vibrational excitations.

Table 1 shows the reference collision cross-section σ_{ref} , reference relative collision velocity v_{ref} , number of internal degrees of freedom v_i , and heat formation for the species.

TABLE 1. Molecular Parameters Used in the Calculations

Species	σ_{ref} cm ²	v_{ref} cm/s	v_i	Heat of Formation kcal/mole
CO ₂	4.33×10^{-15}	1.71×10^5	3.58	-94.10
O	1.75×10^{-15}	2.49×10^5	0.00	59.60
H	1.03×10^{-15}	1.09×10^6	0.00	52.0
CO ₂ (4.3)	4.33×10^{-15}	1.71×10^5	3.58	-87.39
CO(4.7)	3.46×10^{-15}	2.09×10^5	2.00	-20.29
O ₂	3.17×10^{-15}	1.98×10^5	3.60	0.0
OH(2.7)	1.77×10^{-15}	8.00×10^5	2.00	9.4

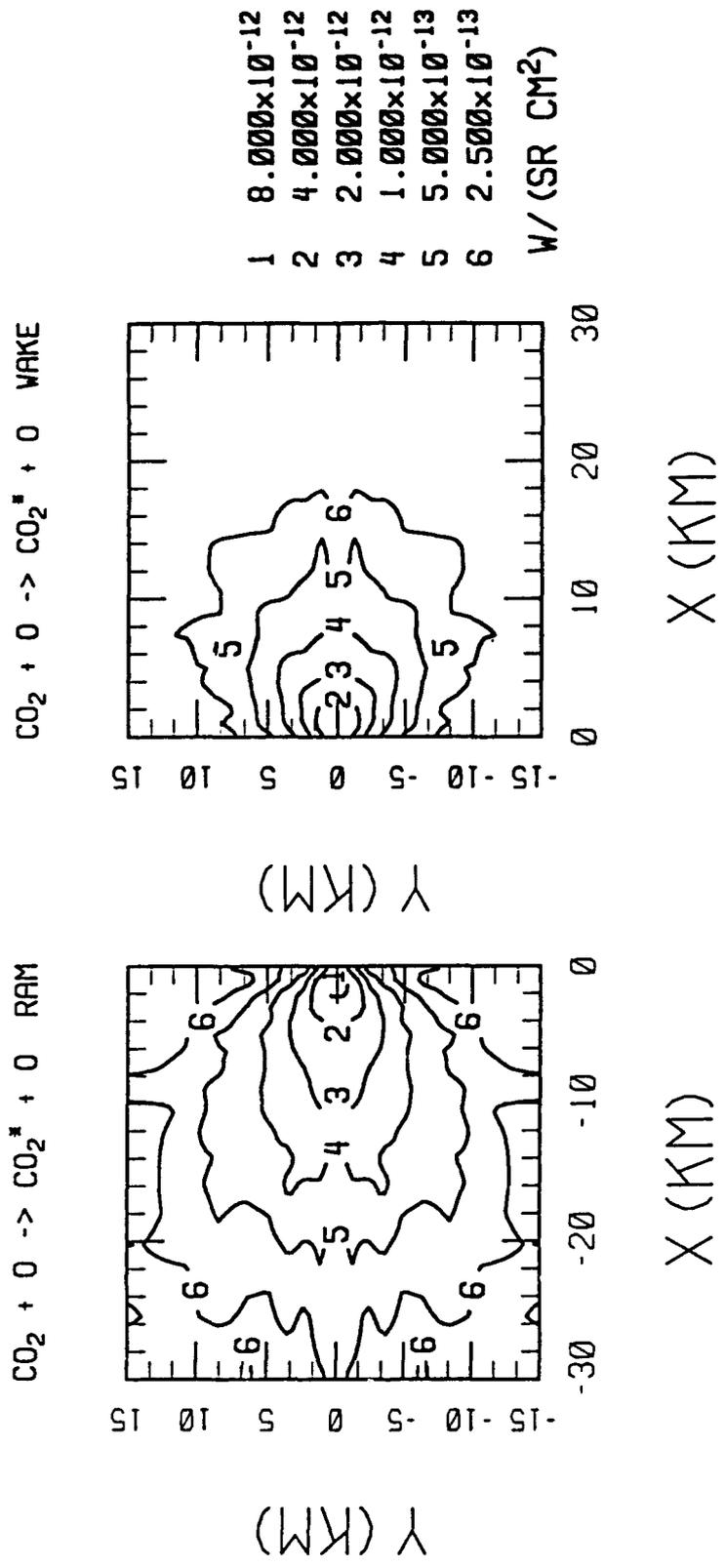
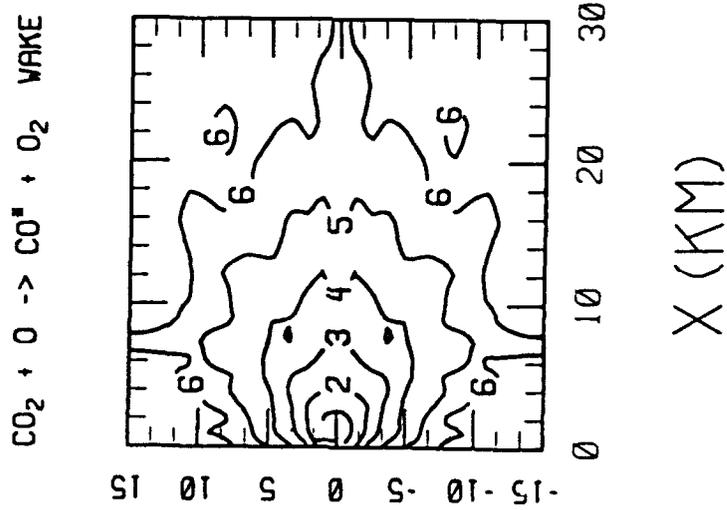
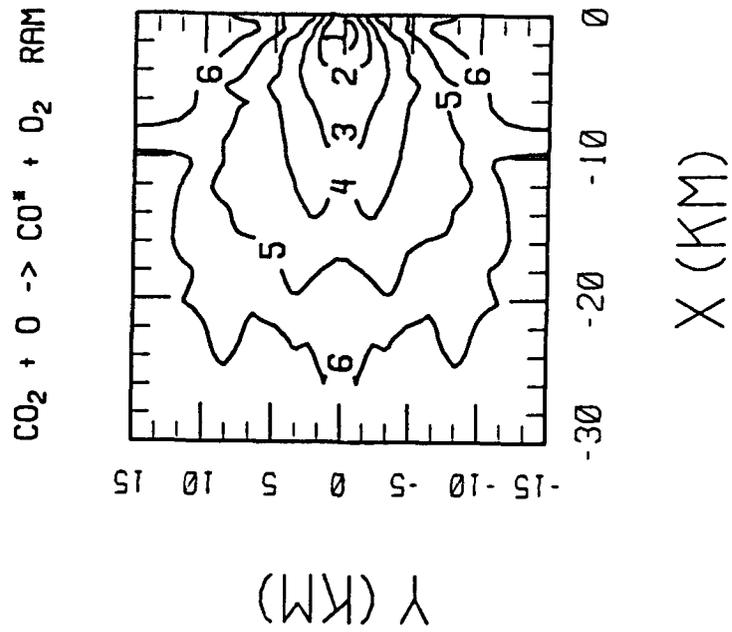


Figure 1. Contour plots showing the CO₂ vibrational excitations at 4.3 μm.



- 1 8.000x10⁻¹¹
 - 2 4.000x10⁻¹¹
 - 3 2.000x10⁻¹¹
 - 4 1.000x10⁻¹¹
 - 5 5.000x10⁻¹²
 - 6 2.500x10⁻¹²
- W/ (SR CM²)

Figure 2. Contour plots showing the CO vibrational excitations at 4.7 μm.

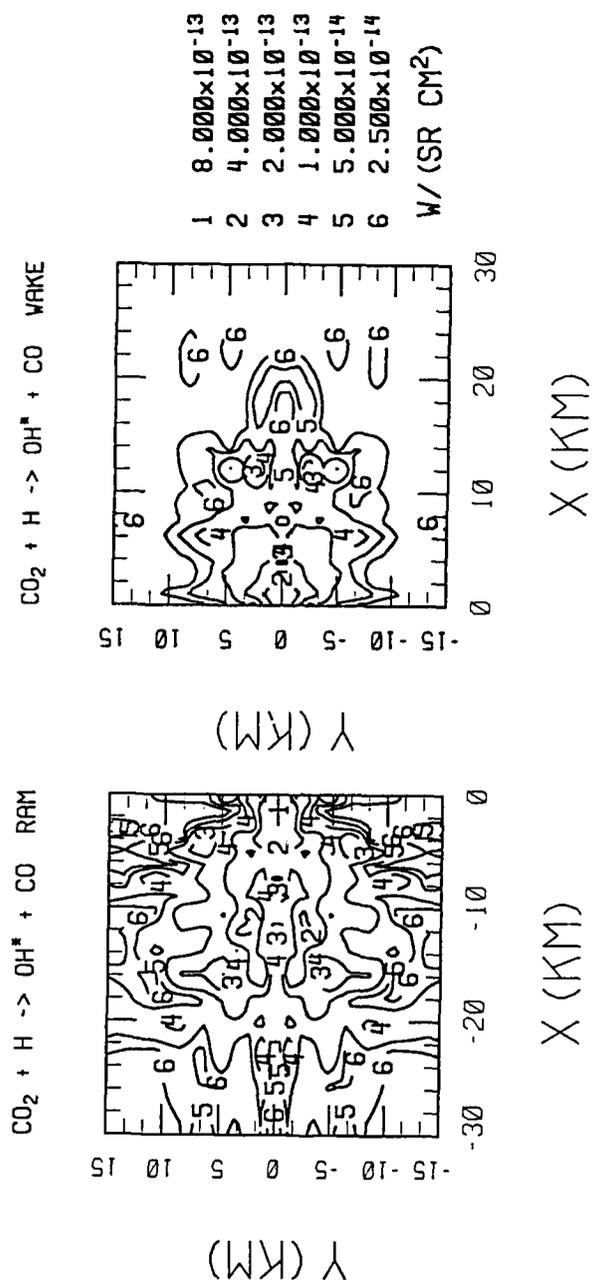


Figure 3. Contour plots showing the OH vibrational excitations at 2.7 μm.

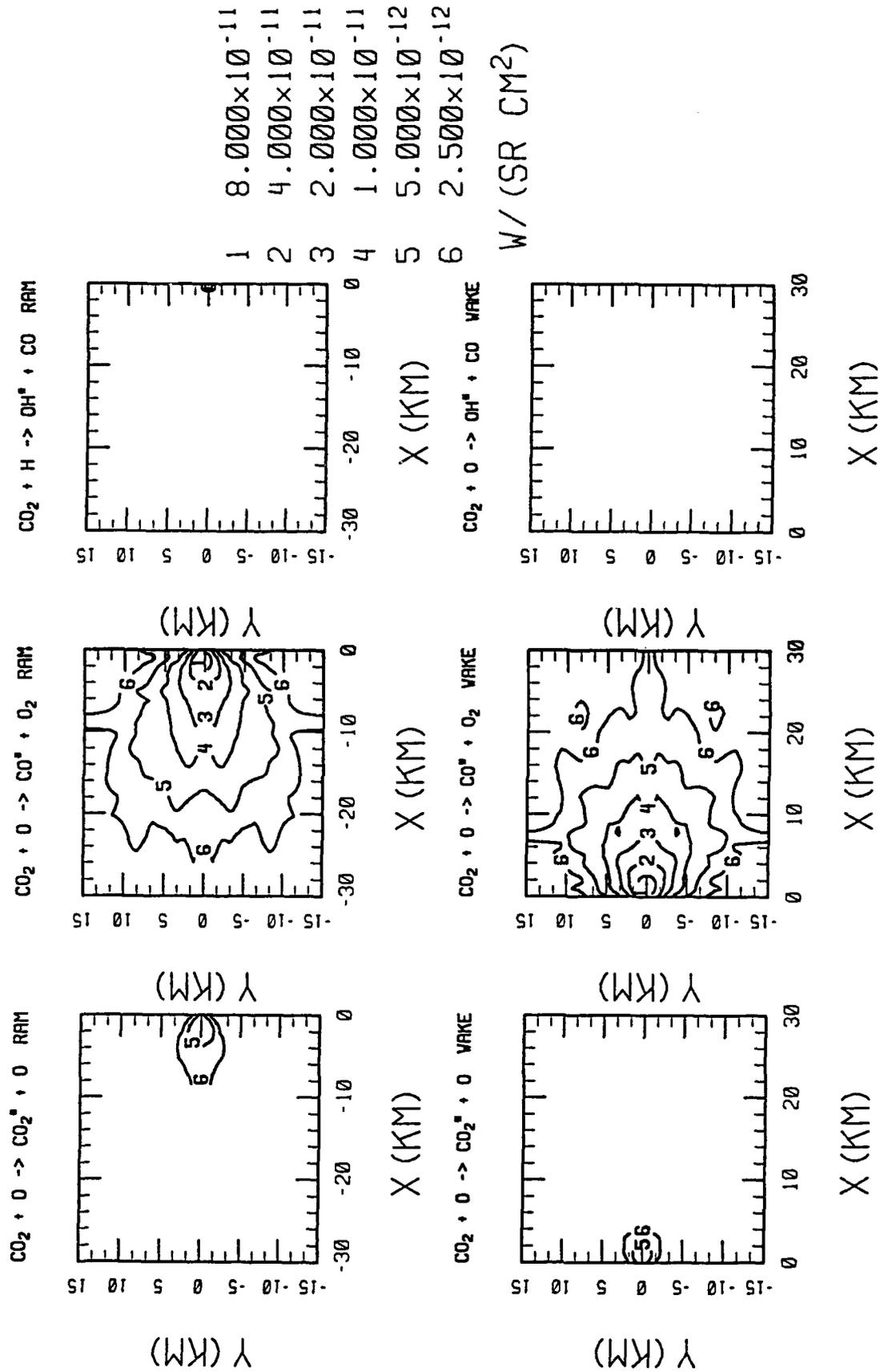
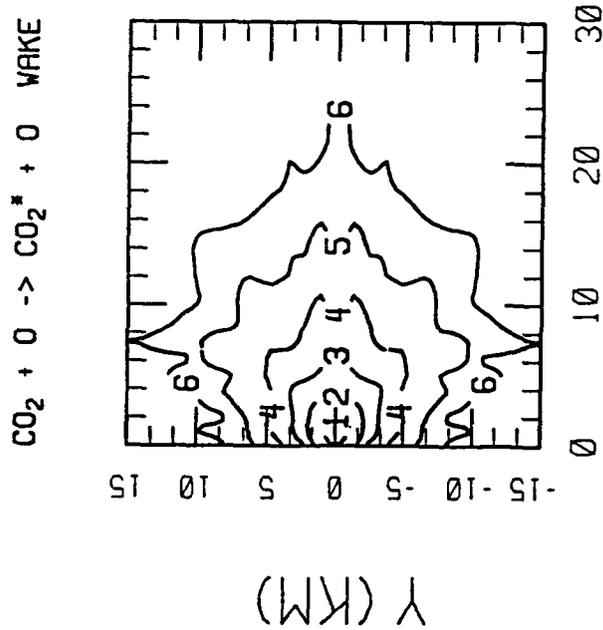
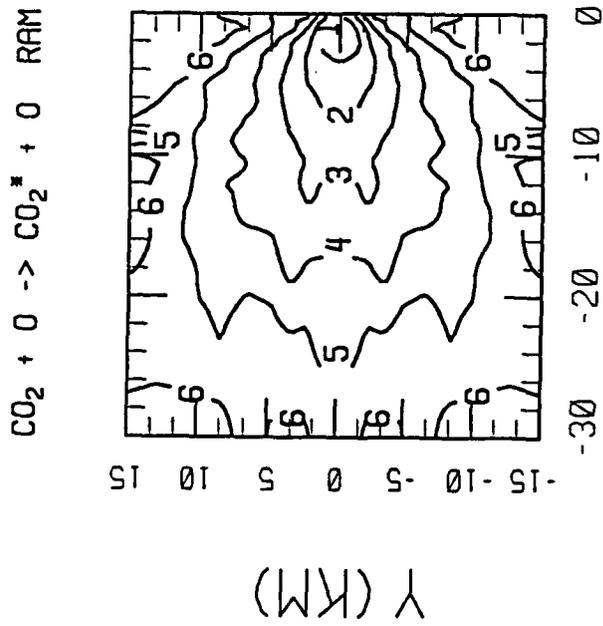


Figure 4. Contour plots showing the CO₂, CO, and OH vibrational excitations for the same scale.



- 1 1.600×10^9
- 2 8.000×10^8
- 3 4.000×10^8
- 4 2.000×10^8
- 5 1.000×10^8
- 6 5.000×10^7

REACTIONS/ (SEC CM²)

Figure 5. Contour plots showing the CO₂ reaction rates.

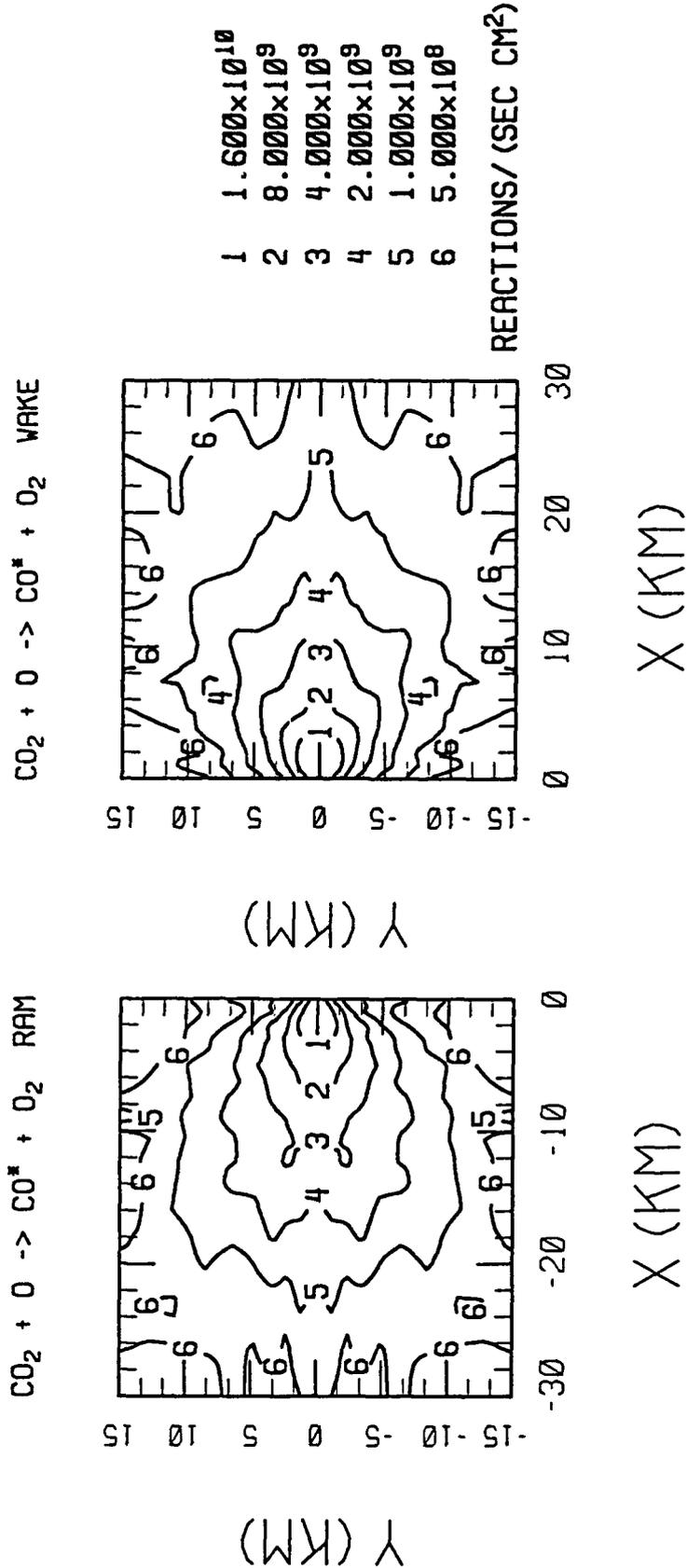


Figure 6. Contour plots showing the CO reaction rates.

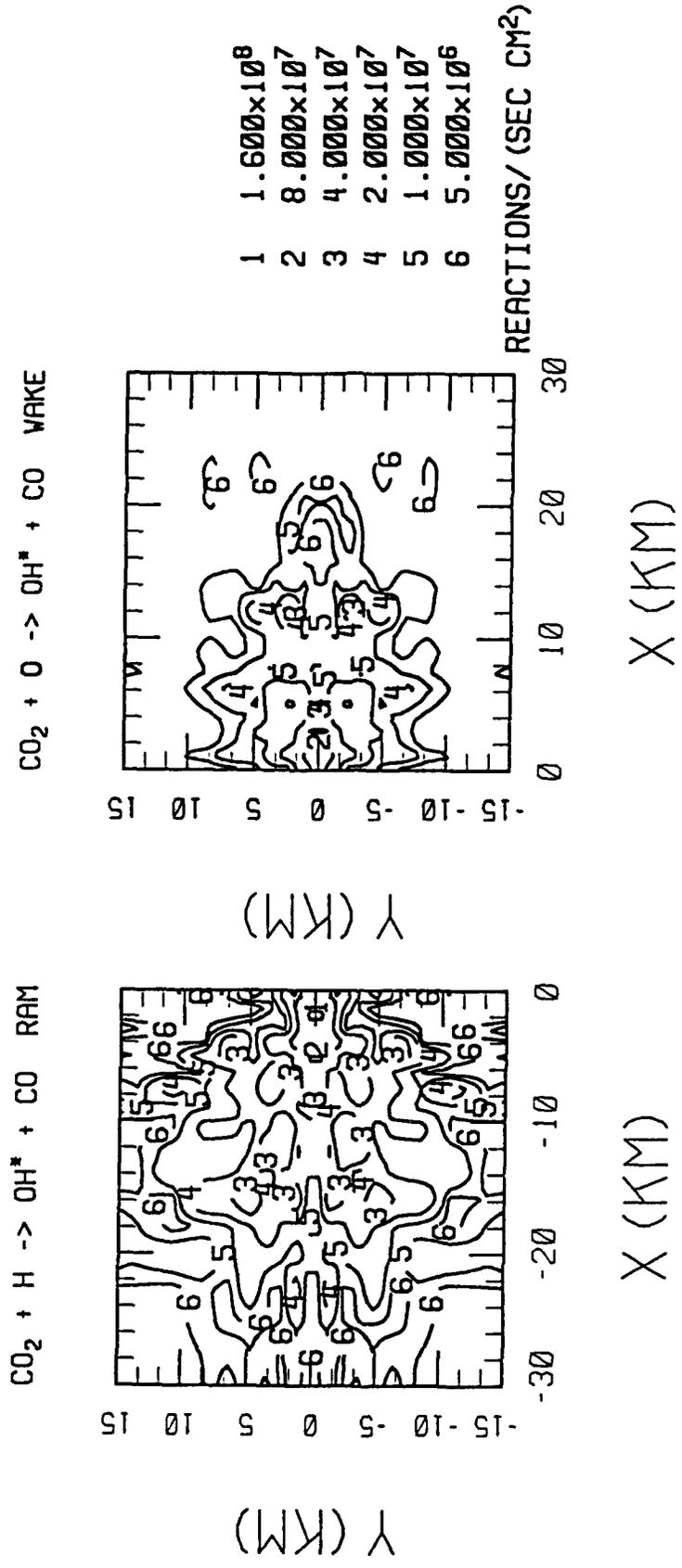


Figure 7. Contour plots showing the OH reaction rates.

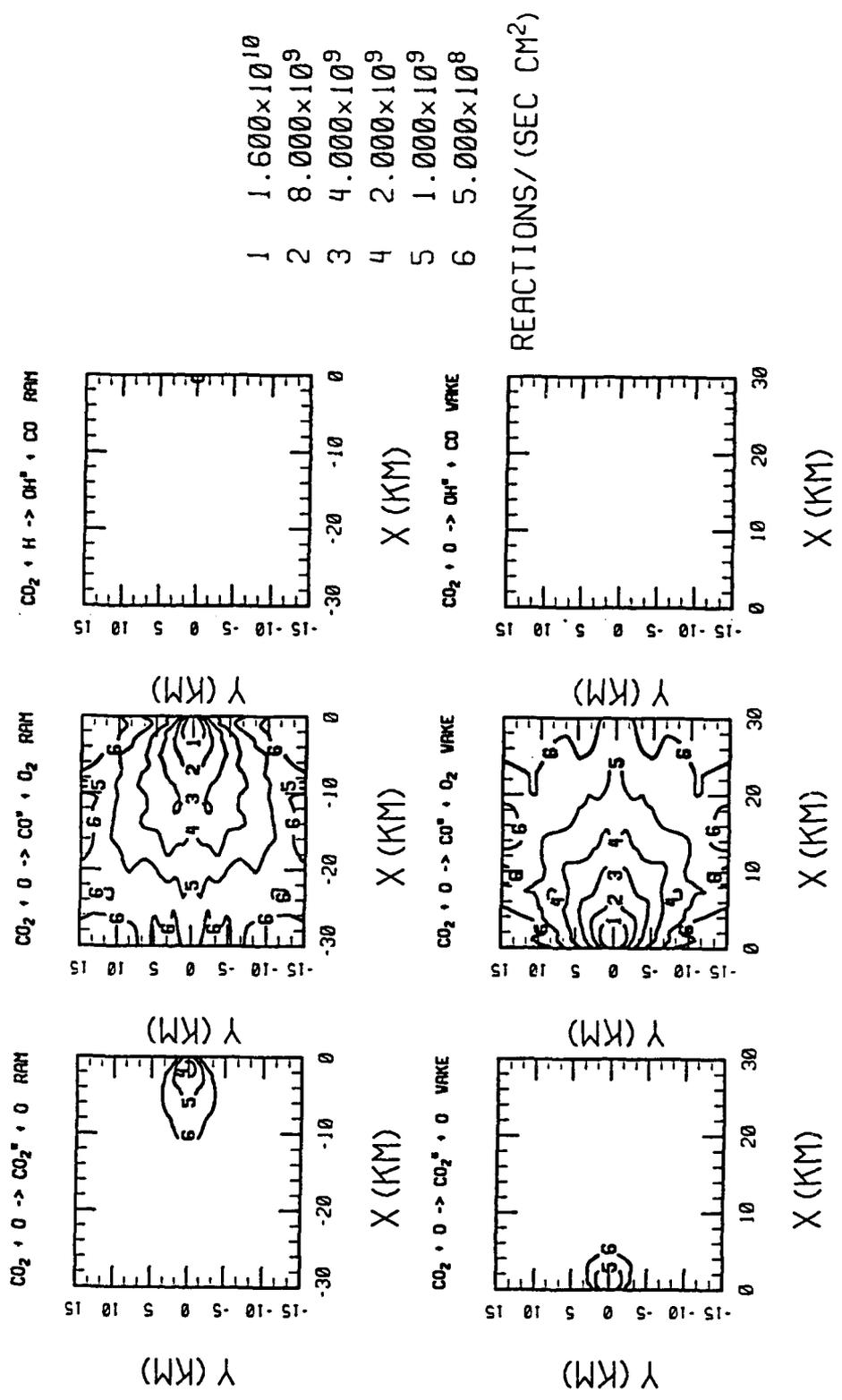
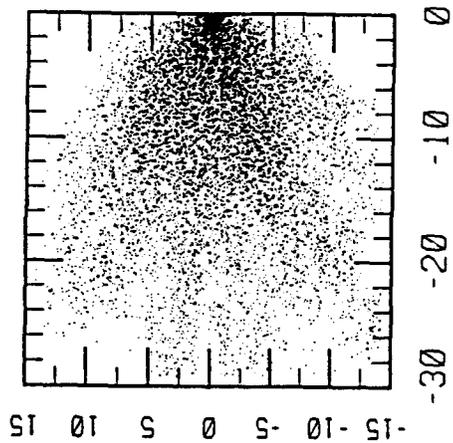


Figure 8. Contour plots showing the CO₂, CO, and OH reaction rates for the same scale.

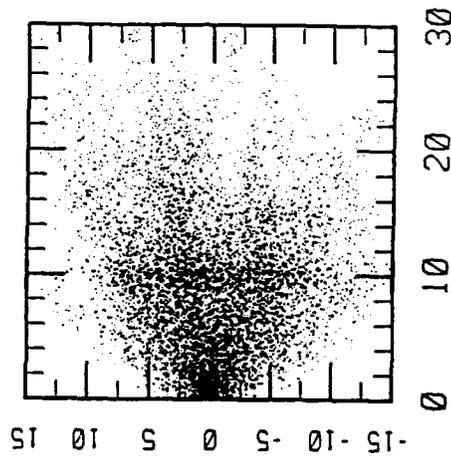
800 KM WAKE



Z (KM)

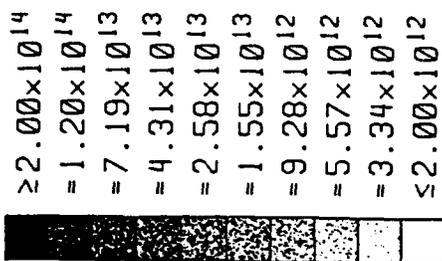
X (KM)

800 KM RAM



Z (KM)

X (KM)



MOLECULES/CM²

Figure 9. Gray scale plots showing the intensity of CO₂ at the time of release.

Table 2 shows the values used in Arrhenius Rate Coefficients for the different reactions, where A, n, and k are constant parameters, T is temperature, and E_a is the activation energy.

TABLE 2. Rate Coefficient Used in SOCRATES, $k = A T^n \exp(-E_a/kT)$

Reaction	A	n	E_a (kcal/mole)
$O_{fast} + CO_2 \rightarrow CO_2(v) + O_{slow}$	3.9×10^{-20}	1.8	6.71
$O_{fast} + CO_2 \rightarrow CO(v) + O_2$	5.6×10^{-11}	0.0	14.21
$H_{fast} + CO_2 \rightarrow CO + OH(v)$	2.5×10^{-10}	0.0	26.43

Table 3 lists the other parameters that have been used in SOCRATES to simulate CO_2 released from a 5 mm diameter nozzle with a mass flow rate of 144 g/s.

TABLE 3. Parameters Used in the Simulations

Atmospheric Temperature	1002.3°K
Atmospheric Number density	$2.047 \times 10^6 \text{ cm}^{-3}$
Altitude	800 km
Mass Flow	144.0 g/s
Exit Plane Area	$2.5 \times 10^{-1} \text{ cm}^2$
Ratio of Specific Heat	1.30
Exit Mach Number	1.40
Exit Nozzle Half Angle	22.5 degrees
Exit Plane Density	$1.789 \times 10^{-2} \text{ g/cm}^3$
Exit Plane Number Density	$2.448 \times 10^{20} \text{ molecules/cm}^3$
Exit Plane Velocity	410.0 m/s
Exit Plane Speed of Sound	$2.929 \times 10^4 \text{ cm/s}$
Exit Plane Temperature	350.0°K
Exit Plane Pressure	$1.18 \times 10^7 \text{ dyne/cm}^2$
Stagnation Temperature	451.9°K
Stagnation Pressure	$3.607 \times 10^7 \text{ dyne/cm}^2$
Thrust	18.5 lb
Velocity of Spacecraft	7.4 km/s

Figure 1 shows the emission at $4.3 \mu\text{m}$ from vibrational excitation of CO_2 produced by collisional energy between O atoms and released CO_2 molecules. Figures 2 and 3 show the emission from the reactive collisions between CO_2 and O and H atoms, respectively. Figure 2, the CO^* emission at $4.7 \mu\text{m}$, shows one order of magnitude higher rate of emission with respect to CO_2^* in Figure 1. This is because the radiative lifetime of CO^* is of the order of μs compared with CO_2^* whose radiative lifetime is of the order of ms. The emission rate of OH^* at $2.7 \mu\text{m}$ in Figure 3, is smaller than the rates of CO^* and CO_2^* (Figures 1 and 2). The rate coefficient given in Table 2 was used to calculate the contours in Figures 1 and 2. The contour plots shown in the figures are in the two directions of ram and wake, where in the ram direction, the flow has a relatively larger initial upstream velocity component, and this contributes to higher-energy collisions; hence, higher levels of emission are produced. Figure 4 is a combination of the plots of Figures 1, 2, and 3 with the same scale for the energy levels. As it is seen in this figure, the emission rate (watts per steradian per cm^2), of CO^* is much higher than that of CO_2^* and OH^* .

Figures 5, 6, and 7 show the reaction rate per sec per cm^2 for reactions 4, 5 and 6. As expected, the intensity of the reactions are similar to those of the emissions in Figures 1, 2, and 3, respectively. Figure 8 represents the combination of the reaction rates in Figures 5, 6, and 7, which is plotted with the same scale. As it is seen, the intensity in reaction 5 for CO^* is much higher than for CO_2^* and OH^* in reactions 4 and 6, respectively. Figure 9 represents the intensity of CO_2 molecule distributions per cm^2 at the time of release, in the two directions of ram and wake.

5. SUMMARY AND CONCLUSIONS

A bundle of CO_2 gas was assumed to be released from a nozzle with a small diameter at high altitude. The diameter of the nozzle and mass flow rate are assumed to be 5 mm and 144 g/s, respectively, in this parametric investigation. The reactions $\text{O} + \text{CO}_2 \rightarrow \text{CO}_2(v) + \text{O}$, $\text{O} + \text{CO}_2 \rightarrow \text{CO}(v) + \text{O}_2$, and $\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}(v)$ were simulated for the above cases from an altitude of 800 km, using the SOCRATES contamination-interaction code. The results were presented in forms of graphs, contour, and gray scale plots for these simulations. These simulations show that the radiation from these reactions should be measurable for the parameters which have been used in these calculations.

6. REFERENCES

- Bird, G. A., "Molecular Gas Dynamics", Clarendon Press, Oxford, 1976.
- Bird, G. A., "Monte-Carlo Simulation in an Engineering Context", Proceeding of the 12th International Symposium on Rarefied Gas Dynamics, Prog. Astronaut. Aeronaut., Vol. 74, pages 239-255, 1981.
- Borgnakke, C., and P. S. Larsen, "Statistical Collision Model for Monte Carlo Simulation of Polyatomic Gas Mixture", Journal of Computational Physics, Vol. 18, pages 405-420, 1975.
- Elgin, J. B., D. C. Cooke, M. F. Tautz, and E. Murad, "Modeling of Atmospherically Induced Gas Phase Optical Contamination From Orbiting Spacecraft", Journal of Geophysical Research, Vol. 95, No. A8, Pages 12197-12208, 1990.
- Elgin, J. B. and R. L. Sundberg, "Model Description for the SOCRATES Contamination Code", Technical Report, AFGL-TR-88-0308, Spectral Sciences, Inc., Burlington, MA 01803, 1988, ADA203154.
- Lai, S. T., E. Murad, and C. P. Pike, "A Proposed Gas Release Experiment on the ARGOS Satellite", Technical Report, PL-TR-92-2058, Environment Research Paper, No. 1098, 1992, ADA256182.
- Lai, S. T., E. Murad, C. P. Pike, W. J. McNeil, and A. Setayesh, "A Feasibility Study on the Xenon and Carbon Dioxide Gas Release Experiments on the ARGOS Satellite", COSPAR, The World Space Conference, Washington, DC, Aug 28-Sept 1, 1992 (Invited Paper).
- Setayesh, A., "A Parametric Study of the Release of CO₂ in Space", Phillips Laboratory, AFSC, Hanscom AFB, PL-TR-91-2052, January, 1991, ADA236271.