Progress Report #8
Final Activity Period: December 1993
H-18070D
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(prepared 1/17/94)

Quantitative Description of Work Performed this period

Efforts this period have focused upon the completion the Line-by-Line radiative transfer model within the IDL environment. Also, this investigator attended and spoke at a December, 20 meeting at MSFC to inform and provide attendees a summary of activities under this purchase order. Herein is the final year-end report under said purchase order. In order to provide the best product to NASA, work efforts have lagged behind schedule in order to obtain the best estimates of the collisional broadening data (ground state atomic and molecular diameters) from Tenn. Tech. University, verify the performance of the code against SPECTRA4, and verify self-absorption performance.

The program SPECTRA5 was implemented in IDL because of the ease and speed with which this could be performed as opposed to FORTRAN or C code. The code is completed in the sense that it will accurately predict UV-VIS emission from the elements contained in the data from the NIST database #24, Scandium through Nickel, subject to the constraints given in the November Progress report under this effort. It should be revised at some point to include selected data from the old NBS monogram 52 on experimentally determined transition probabilities which were used in the SPECTRA4 atomic spectra code. However, at present, the code will predict the important species, Fe, Cr, and Ni using the NIST database #24, which is considered to be the best to date for our purposes.

The primary focus this period has been to perform self-consistency checks and validation against SPECTRA4 and to include adequate documentation with the procedure codes. In particular this means that the optically thick limit, for infinite length of emitting/absorbing gas, has been verified to approach the theoretical black-body emission. And, for future verification, the code will produce the black-body curve for comparison to predicted emission radiance values. In the other extreme, as the gas length becomes very small, the SPECTRA5 was verified to produce the same results as those obtained from SPECTRA4 (i.e. the corrected version of SPECTRA4). The convolution of the instrument response function was verified by performing wavelength integration over a selected line in the optically thin regime and comparing to SPECTRA4.

The issue of the detector response function was resolved. The response function must be integral normalized to unity, similar to the manner in which the absorption coefficient is normalized to the line-strength. This will ensure that the wavelength integrated values of emission result in the proper emission radiance.

The radiative transfer is performed for a single narrow FOV of uniform thermodynamic flow field properties, temperature, and partial pressures, as is suitable for analysis of Mach disc spectral measurements as described in the June AIAA Monterey, CA paper, 'Simulation of UV Atomic Radiation for Application in Exhaust Plume Spectrometry'. This technique inherently assumes no overlapping lines, an assumption which may be invalid under conditions of multiple species and/or high mole-fractions/concentrations. This assumption is examined as part of SPECTRA5 calculations. The appropriate method of dealing with this problem remains to be solved. After running some rather extreme cases, it was found that lines may overlap at the higher species concentrations due to absorption line broadening effects. The significance of these effects has not been addressed, but is generally thought to not be a major problem. Moreover at the concentration levels typical of nominal conditions observed at the Technology Test Bed, overlapping lines are either absent or almost insignificant.

Other than the determination of the correct procedure for implementing the instrument response convolution, no modifications have been performed to the overall scope of the code. Hence the limitations and descriptions provided in the November Progress report under this effort are still applicable.

In summary, the work performed during this contract has accomplished most of the goals of the statement of work and has been conducted and coordinated to closely follow the needs and objectives of EB22 personnel. Basic analytical and numerical research was performed towards developing a working understanding of the radiative transfer mechanisms and equations for predicting atomic radiation from the SSME Mach disc region. Results of these studies demonstrated the importance of self-absorption effects and were reported as required in the aforementioned AIAA conference. Also, studies formed the foundation for implementation of the present LBL code, SPECTRA5, which is now a working model suitable for assisting spectral analysis efforts and most importantly will provide the capability to generate the family of curves for radiant intensity versus specie concentration which can be used to train the AI and Neural Net systems to perform quantitative spectral analysis to determine specie erosion rates for events observed by the OPAD instrumentation. Support has been provided to MSFC EB22, NASA Ames, University of Alabama, and Tenn. Tech. University personnel as needed and as specified in the statement of work. The SPECTRA5 code is available via anonymous ftp to *aedc-vax.af.mil* and consists of the following ascii files: *absorp.pro, line.pro, spectra5.pro, comp.lst* and *element.lst*. The NIST database must be obtained directly from NIST.

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13. ABSTARCT (Maximum 200 words)

The development of an analytical-numerical model to predict radiant emission or absorption is discussed herein. A voigt profile is assumed to predict the spectral qualities of a singlet atomic transition line for atomic species of interest to the OPAD program. The present state of this model is described in each progress report required under contract. Model and code development is guided by experimental data where available. When completed, the model will be used to provide estimates of specie erosion rates from spectral data collected from rocket exhaust plumes or othersources.

Emphasis on brief summary of year's activities and completion of LBL model SPECTRA5

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