NASA/ASEE SUMMER FACULTY FELLOWSHIP PROGRAM

MARSHALL SPACE FLIGHT CENTER
THE UNIVERSITY OF ALABAMA

BIAS AND UNCERTAINTY IN THE ABSORPTION EMISSION

MEASUREMENT OF ATOMIC SODIUM DENSITY IN THE SSME EXIT PLANE

Prepared By:	Leslie E. Bauman
Academic Rank:	Associate Professor and Senior Research Scientist
University and Departments:	Mississippi State University Physics & Astronomy and Diagnostic Instrumentation and Analysis Laboratory

NASA/MSFC:
    Laboratory: Propulsion
    Division: Propulsion Systems
    Branch: Performance Analysis

MSFC Colleague: Dr. Charles F. Schafer

Contract No: NGT-01-002-099
    The University of Alabama

BIAS AND UNCERTAINTY IN THE ABSORPTION EMISSION MEASUREMENT OF ATOMIC SODIUM DENSITY IN THE SSME EXIT PLANE

Leslie E. Bauman*

INTRODUCTION

The measurement of atomic sodium concentration in the TTB 019 firing of April 1990 is significant in that it represents the first measurement of density at the exit plane of the space shuttle main engine (SSME).[1] The knowledge of the sodium density, combined with the certainty that the exit plane of the plume is optically thin at the sodium D-line wavelengths, provides essential information for evaluation of diagnostic techniques using sodium atoms, such as resonant Doppler velocimetry[2] for temperature, pressure, and velocity through high resolution fluorescent lineshape analysis.

The technique used for the sodium atom line transmission (SALT) measurements is that of resonant absorption emission using a hollow cathode lamp as the reference source. The lamp provides narrow band sodium D-line emission as well as nearby neon lines for reference measurements. The reference is essential to account for such effects as fluctuations in the source emission, transmission losses through beamsteering or fog in the path, etc. The detection system is a polychromator, which separates the neon and sodium lines but spectrally integrates the lines.

The SALT measurements were reported at the 1990 Advanced Earth to Orbit Propulsion Conference and are summarized here for clarity. Pre- and post-firing of the engine the reference intensities of the sodium and neon lines were measured; these signals (corrected for background), $I_{Na,0}$ and $I_{Ne,0}$, were stable with a signal-to-noise (S/N) ratio of 600 to 1. During the test, measures were made of the transmitted signals, $I_{Na,t}$ and $I_{Ne,t}$, as well as the lamp-off emission/background signals, $B_{Na,t}$ and $B_{Ne,t}$ with an effective time resolution of 1 second. The transmission, T, is found then as

$$T = \frac{I_{Ne,0}\, I_{Na,t} - B_{Na,t}}{I_{Na,0}\, I_{Ne,t} - B_{Ne,t}} \quad . \tag{1}$$

Through the use of TDK predictions of temperature and density for the flight engine case and radiative transfer calculations, this line-of-sight, spectrally integrated transmission indicates a sodium atom concentration, i.e. mole fraction, of 0.91e-10. The calculation does assume a sodium constant mole fraction across the plume and since the sodium is present in the cryogenic fuel, the assumption of uniform distribution across the plume seems well founded.

But tied into the calculation are also assumptions and measurement uncertainties that are the subject of this paper. Because of the narrow shape of the source emission, the uncertainties in the absorption profile could introduce considerable bias in the measurement. The following were investigated as part of this work: (1) the inclusion of hyperfine splitting[3] of the D-lines in the calculation, (2) the use of the flight engine predictions of plume temperature and density versus those for the large throat engine (The engine for the TTB 019 firing was actually the large throat engine but the large throat TDK data was not available and the flight engine data was used.), (3) the assumption of a

---
*Mailing Address: P.O. Box 5167, Mississippi State, MS 39762.
Phone: (601) 325-2806. Fax: (601) 325-8465.

Gaussian, i.e. Doppler, distribution for the source radiance with a temperature of 400 K, (4) the use atomic collisional shift and width values from the work by Jongerius,[4] and (5) a Doppler shift from a 7t outward velocity vector at the plume edge.

Also included in the study was the bias introduced by an uncertainty in the measurement of the D1/D2 line ratio in the source. When this ratio was observed to deviate from that predicted by equilibrium statistics, additional complexity was added to the system in the form of an optical multi-channel analyzer in order to track the ratio between the source sodium D1 and D2 line emissions.

CALCULATIONS

Numeric Calculations. A computer program was written to perform the numerical integration of the radiative transfer equation to solve for the spectral plume radiance, B_ν, plume optical depth, τ_ν, and source radiance, I_ν, given inputs of the plume temperature, water and hydrogen densities, and velocity as functions of the beam path across the plume. The absorption line was modeled as a Voigt function[5] using the calculations of Humlicek.[6] This function which arises from a classical impact theory of line broadening has its limitations but is an accurate model for the regime of these measurements. The assumption used by Dobson and Eskridge (DE) to model the source radiance as a Gaussian function, i.e. including Doppler broadening only, was retained. This is valid only since the plume is optically thin; if the absorption were stronger the wings of the source function would become important and a Voigt model including the natural width of the line should be used. (Ideally, when appropriate equipment is available, the spectrum of the source should be measured.) The calculation includes overlap of the D1 and D2 lines as well as the hyperfine lines. The transmission is then found from spectral integrations over the D1 and D2 line regions where the source function is significant,

$$T = \frac{\int_{D1} I_\nu \exp(-\tau_\nu)d\nu + F \int_{D2} I_\nu \exp(-\tau_\nu)d\nu}{\int_{D1} I_\nu \, d\nu + F \int_{D2} I_\nu \, d\nu} , \qquad (2)$$

where F is the measured deviation from equilibrium for the D1 to D2 lamp emission ratio. The negative natural logarithm of the transmission is an effective optical depth for the combined lines, τ_{Na}, and is linear with the sodium mole fraction at the low densities of the SSME plume, so that the desired sodium mole fraction, [Na], can be found from the measured transmission through the constant C found from numerical calculations as [Na] = C τ_{Na}. The biases and uncertainties in the measurement were studied by solving for the constant C for a range of sodium concentrations.

Approximate Calculation. In the limit that the lamp lineshape is infinitely narrow and collisional or Doppler induced lineshifts are negligible, one can calculate the effective optical depth as

$$\tau_{D1 \text{ or } D2} \approx 3.28e\text{-}10 \, [Na] \, f_{D1 \text{ or } D2} \int_{plume} N \, T^{-\frac{1}{2}} \, dx , \qquad (4)$$

where f is the dimensionless oscillator strength, N is the plume density in molecules/cm^3, and T is the plume temperature in Kelvin. While this approximation may not provide an accurate absolute measure of the sodium concentration, it allows inspection of the bias from the use of TDK predictions in the calculations.

RESULTS

As a test case, numerical calculations were performed on the flight engine data with the same assumptions as used by DE, i.e. no hyperfine splitting, no Doppler shift and the same Jongerius shift and width values. A sodium concentration of 0.88e-10 was determined (C = 1.45e-9). This compares to the results of DE of [Na] = 0.91e-10. As the calculations were performed with different Voigt schemes and different numerical integration schemes, the agreement seemed acceptable.

Hyperfine Splitting. There is a significant error from neglecting hyperfine splitting. For the flight engine data, the addition of hyperfine splitting to the model gives C = 1.75e-9, an increase of 20%.

Large Throat. The integral of the plume density divided by the square root of temperature is 18% higher for the large throat predictions compared to those for the flight engine and a consequent decrease in the calculated sodium concentration was expected. A value of 0.88e-10 was determined (C = 1.44e-9), serendipitously canceling the effect of inclusion of hyperfine splitting -- the bias from using the TDK predictions for the flight engine rather than the large throat engine is about 20%.

Source Line Width. Varying the source temperature by æ100K changes the Doppler width of the sodium lines by approximately æ12%. The bias in the calculated sodium concentration was only 5% for the entire range.

Doppler Shift. With only the suggestion that the plume velocity vector is 7° outward at the plume edge, it was necessary to construct a model for the outward velocity component. I chose a model that tapered this outward component down to zero at the position of the shock through a square root relationship to the proportional distance out from the shock. The central region of the plume shows a negligible line shift, the far region has a small red shift and the near region has a small blue shift. The net effect is to slightly lower the absorption at line center leading to an increased value for the sodium concentration. For the chosen model the sodium concentration was found to be 0.90e-10, a 2% bias. If an outward velocity is present at the measurement position, ignoring the Doppler shift will bias the measurements to a lower concentration than actual.

Collisional Shift and Width. Using the error limits given by Jongerius[4] variations in the width gave a 5% variation in the calculated sodium concentration. Variations in the line shifts did not measurably affect the calculations.

Lamp D1 to D2 Ratio. Varying this measurement parameter over 10% leads to a variation in sodium concentration of 3%.

Combining these last four uncertainties in a square root of the sum of the squares fashion gives a combined uncertainty of less than 10% for the sodium concentration. The hyperfine splitting can easily be kept in the model at the expense of computing time so this bias should not be included in the combination and hopefully the TDK calculations are accurate enough to not add appreciable error. This ±10% uncertainty is small compared to the measurement uncertainty of nearly ±40%.

CONCLUSIONS AND SUGGESTIONS

One question that I had about the SALT measurements was that since the integrated line strengths are well known, why not use a broadband source where there would be no bias due to lack of information about lineshapes or shifts? The answer is that compared to the

precision of the SALT measurements, the biases introduced by uncertainties in lineshapes and shifts are not important. And, the wavelength regions would need to be narrowly set on the sodium lines or small uncertainties in the measured intensities would amplifying the uncertainty in the measured sodium concentration. In my estimation, the SALT technique as applied to the TTB is a good one.

I do however have two suggestions for improving the measurement precision. The first involves the data collection scheme and in particular time averaging. A useful rule of thumb for experimentalists is to average the most fundamental property. In the case of the SALT measurements, the fundamental property is the optical depth, directly proportional to the sodium concentration, and because of the optical thinness of the plume very nearly one minus the transmission. So ideally, one should time-average the transmission measurement, i.e. the sodium to neon intensity ratio, rather than time averaging the intensities as is done with the SALT data collection.

In a simple look at the fluctuations, if the important fluctuations are those of the sodium optical depth and broadband transmission and source effects, lumped together as A, then

$$\langle I_{Ne,t} \rangle_t = (\bar{A} \pm \delta A)\, I_{Ne,0} \qquad (5)$$

and

$$\langle I_{Na,t} \rangle_t = (\bar{A} \pm \delta A) I_{Na,0} \exp[-(\bar{\tau} \pm \delta\tau)] . \qquad (6)$$

Then ratioing the time-averaged signals will give

$$T_{avg} \approx (1 \pm 2\,\delta A/\bar{A}) \exp[-(\bar{\tau} \pm \delta\tau)] , \qquad (7)$$

essentially doubling the uncertainty due to the time varying broadband transmission factor. On the other hand, if the instrument time response is fast enough to resolve the fluctuations, then averaging the ratio of the sodium and neon signals will remove this uncertainty.

My other suggestion is to double pass the SALT beam, doubling the measured optical depth. If this can be done without a concommitent increase in the measured transmission uncertainty, then the uncertainty in the sodium concentration will be halved. The uncertainty would be expected to increase because of beam transmission effects, but I would not expect it to double and the uncertainty would need to double in order to cancel the benefits of the double pass operation. The adoption of both of these suggestions will, I believe, lead to a better measurement of the SSME plume atomic sodium density.

REFERENCES
1. Dobson, C.C., Eskridge, R.H., "Resonant Absorption and Emission Measurements of Atomic Sodium in the SSME Exit Plane," Advanced Earth to Orbit Propulsion Conference, Huntsville, AL, 1990.
2. Zimmermann, M., and Miles, R.B., Appl. Phys. Lett., 37, 885, 1981.
3. Fairbank Jr., W.M., H nsch, T.W., and Schawlow, A.L., J. Opt. Soc. Amer., 65, 199, 1975.
4. Jongerius, M.J., Van Bergen, A.R.D., Hollander, TJ., and Alkemade, C. Th. J., J. Quant. Spectrosc. Radiat. Transfer, 25, 1, 1981.
5. Mitchell, A.C.G., Zemansky, M.W., Resonance Radiation and Excited Atoms, Cambridge Press, London, 1971.
6. Humlicek, J., J. Quant. Spectrosc. Radiat. Transfer, 27, 437, 1982.