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Shuttle Upper Atmosphere Mass Spectrometer Experimental Flight Results

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Calibrated pressure measurements for species with mass-to-charge ratios up to 50 amu/e⁻ were obtained from the shuttle upper atmosphere mass spectrometer experiment during re-entry on the STS-35 mission. The principal experimental objective is to obtain measurements of freestream density in the hypersonic rarefied flow regime. Data were collected from 180 to about 87 km. However, data above 115 km were contaminated from a source of gas emanating from pressure transducers connected in parallel to the mass spectrometer. At lower altitudes, the pressure transducer data are compared to the mass spectrometer total pressure with excellent agreement. Near the orifice entrance, a significant amount of CO₂ was generated from chemical reactions. The freestream density in the rarefied flow flight regime is calculated using an orifice pressure coefficient model based upon direct simulation Monte Carlo results. This density, when compared with the 1976 U.S. Standard Atmosphere model, exhibits the wavelike nature seen on previous flights using accelerometry. Selected spectra are presented at higher altitudes (320 km) showing the effects of the ingestion of gases from a forward fuselage fuel dump.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>amu/e⁻</td>
<td>atomic mass unit per unit charge</td>
</tr>
<tr>
<td>((C_p))_i</td>
<td>equilibrium pressure [see Eq. (2)]</td>
</tr>
<tr>
<td>C1, C2</td>
<td>inlet system flow restrictors (i.e., leaks)</td>
</tr>
<tr>
<td>F_i</td>
<td>mole fraction of species i</td>
</tr>
<tr>
<td>I_i</td>
<td>inlet current of species i, A</td>
</tr>
<tr>
<td>k_o</td>
<td>range valve constant; 140.0 for range valve closed or 1.0 for range valve open</td>
</tr>
<tr>
<td>P_i</td>
<td>pressure of species i, N/m²</td>
</tr>
<tr>
<td>P_r</td>
<td>equilibrium pressure, N/m²</td>
</tr>
<tr>
<td>P_s</td>
<td>surface pressure, N/m²</td>
</tr>
<tr>
<td>P_t</td>
<td>total pressure due to all species, N/m²</td>
</tr>
<tr>
<td>q_∞</td>
<td>freestream dynamic pressure (i.e., (1/2)pV²), N/m²</td>
</tr>
<tr>
<td>S_i</td>
<td>sensitivity coefficient of species i, A/N/m²</td>
</tr>
<tr>
<td>x, y, z</td>
<td>body axes</td>
</tr>
<tr>
<td>V</td>
<td>velocity, m/s</td>
</tr>
<tr>
<td>V1, V2, V3</td>
<td>inlet valve, dynamic range valve, and protection valve, respectively</td>
</tr>
<tr>
<td>α</td>
<td>angle of attack, deg</td>
</tr>
<tr>
<td>β</td>
<td>sideslip angle, deg</td>
</tr>
<tr>
<td>ρ</td>
<td>density, kg/m³</td>
</tr>
<tr>
<td>τ</td>
<td>change in pressure of species i due to chemical reactions, N/m²</td>
</tr>
</tbody>
</table>

Introduction

The main objective of the shuttle upper atmosphere mass spectrometer (SUMS) experiment is to obtain measurements of freestream density in the hypersonic, rarefied flow regime during the Shuttle atmospheric re-entry. These measurements, when combined with acceleration measurements, allow the determination of Orbiter aerodynamic coefficients in a flow regime previously inaccessible to experimental techniques. This report presents the results of analysis of flight data from the SUMS experiment taken during the Orbiter’s re-entry on the STS-35 mission. A complete description of the SUMS experiment is given in Ref. 1. Detailed drawings of the flight and laboratory equipment including dimensions, calibrations, and other laboratory procedures are given in Ref. 2. A brief review is given here for clarity.

Experiment Description

The main elements of the SUMS flight equipment consist of a pressure transducer (689.476 N/m² or 0.1 psia), an inlet system, and a flight mass spectrometer. As depicted in Fig. 1, the pressure transducer is in parallel with the inlet system, and it provides back-up protection to the mass spectrometer in the event of valve closure failures, as well as a source of independent pressure data to compare with the mass spectrometer data. It is important to note that two additional pressure transducers from a different experiment were connected to the same orifice for a total of three transducers connected in parallel with the mass spectrometer.

The inlet system includes stainless steel tubing connecting a filter, an inlet valve, large and small calibrated pinched tube leaks in parallel (see C1 and C2 in Fig. 1), and a dynamic range valve. When the dynamic range valve closes, the gasflows exclusively through leak C2, thereby expanding the measurement range. The mass spectrometer is located remotely from the inlet system within a pressure housing that is filled with sulfur hexafluoride at 1.0 atm pressure. A protection valve is placed in the gas line to the mass spectrometer as a backup to an inlet valve failure. The physical arrangement of the SUMS components on the Orbiter is shown schematically in Fig. 2. Inlet tubing penetrates the Orbiter chin panel just aft of the nose cap and connects to the inlet system after passing through the nose wheelwell bulkhead. The inlet system is connected with another tube to the mass spectrometer, which is mounted on the nose wheelwell bulkhead (Fig. 2). The inlet orifice size and all relevant tubing lengths are given in the schematic, Fig. 3. The inlet orifice is constructed from Columbium (Niobium) because of its high melting point and resistance to corrosion at high temperatures. This port also serves as a common gas inlet for 2 of the 36 pressure transducers that comprise the shuttle entry air data system (SEADS) experiment. The internal tubing is constructed from stainless steel. Temperature measurements from a sensor located in the inlet box.

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indicated a constant temperature of about 12°C during the flight. A more complete description of all of the components can be found in Ref. 2. Data taken during flight are stored on a remotely located tape recorder and downloaded after the Shuttle flight.

The SUMS mass spectrometer is a flight spare from the Viking (Mars mission) project upper atmosphere mass spectrometer (UAMS) experiment that has been modified to provide mechanical, electrical, and data compatibility with the Shuttle. SUMS experiment operation during flight is controlled by commands stored in the Shuttle computer and by internal "firmware" logic. The application of power for vacuum maintenance and for normal equipment operation is controlled by stored Shuttle commands, and internal operations, such as opening and closing valves, are performed by the SUMS control electronics, which depend upon atmospheric conditions as measured by the SUMS pressure transducer and/or mass spectrometer.

The mass spectrometer has a mass range of 1–50 amu/e− in increments of 0.25 amu/e− and can measure the gases hydrogen (H2) through carbon dioxide (CO2) at a rate of 1 scan every 5 s. One typical 5 s SUMS measurement scan obtained near 90 km altitude during STS-35 is shown in Fig. 4. SUMS is powered on shortly before the initiation of de-orbit burn, and then samples the inlet gases with the range valve open until an altitude of about 108 km is reached. At that point, the range valve closes leaving only the small leak to transmit gas to the mass spectrometer until about 87 km. Below 87 km, the inlet valve closes, but the mass spectrometer continues to operate until landing to observe the system decay characteristics as it is pumped down. The complete re-entry data set on STS-35 consists of approximately 760 scans representing about a 4000 s measurement time interval. The freestream gas flow relative to the orifice is at an angle of −29 deg when the Orbiter is at the nominal re-entry angle of attack of 40 deg.

**SUMS System Calibration**

**Laboratory Tests**

Calibration of the instrument was accomplished in the laboratory using a setup of specially designed ground support equipment (GSE) connected to the flight hardware. Calibration includes introducing a test gas to the GSE and varying pressure statically (i.e., set a pressure and hold) as well as dynamically (i.e., vary pressure with time). The dynamic test setup provides a method to simulate pressure changes expected during flight. Inlet pressures are then measured (using a sensitive Baretron pressure gauge) and compared to the resulting ion current peaks measured by the mass spectrometer itself. The ion current, when divided by inlet pressure, provides the sensitivity coefficients (amps/torr) of individual gases (e.g., N2, CO, O2, and CO2) connected to the inlet test setup. This procedure allows the partial inlet pressure of each species to be determined from a measured ion current in the mass spectrometer during flight. Currents were also recorded for peaks that resulted from the double ionization or "cracking" of a molecule. Examples of these measurements include the ion current peak measured at 14 from doubly ionized N2 and the ion current peak measured at 28 and 16 as CO dissociates and ionizes into CO+ and O+.

Knowledge of the doubly ionized to singly ionized current ratios and the cracking patterns allows the determination of the amount that each species contributes to a particular peak, which is necessary for calculating the correct composition of the gas as it enters the mass spectrometer. These ratios are specific to the SUMS instrument, and the important ones are listed in Table 1.

**System Response Function**

A change in gas pressure at the inlet is not sensed immediately by the mass spectrometer because a time lag response exists caused by the enclosed volumes and tube lengths. During some time interval when the descent rate of the Orbiter is fairly constant, the time lag can also be expressed as an altitude shift. Consideration of the shift is most important when SUMS data must be combined with, or compared to, other data. For example, to compare the SUMS...
ambient density predictions to the 1976 U.S. Standard Atmosphere, it would be necessary to account for the system response time.

An electrical network analog was developed to predict the sensor lag or response function of the SUMS system. The conductances of the inlet tubing and the UAMS terminator were modeled as resistive elements; the volumes of the system were modeled as capacitive elements, and the time-dependent input pressure was modeled as an applied voltage. The coefficients of the solutions to the differential equations describing the electrical network model were obtained from a series of static and dynamic calibration laboratory tests of the flight equipment. A volume that represents the tubing forward of the inlet system was used during the tests. However, this laboratory setup did not physically include the two flight pressure transducers that are connected in parallel to the inlet line. Attempts to apply the electrical analog model results for the system as flown were unsuccessful because air, which was trapped behind the filter of each pressure transducer, slowly leaked into the system. This effect could not be satisfactorily adapted to the preflight system response model results because of the lack of knowledge of the characteristics of the phenomena. Therefore, the electrical analog model proved to be of little practical use for postflight estimates of the time lags. However, pressure transducer flight data did allow an experimental determination of the pressure lag for the range valve closed condition.

**Estimate of the System Response**

**SUMS Time Lag**

The SUMS measurement time lag can be determined from the pressure transducer output for the range valve closed condition. The correlation with the pressure measurements requires the calculation of total pressure using the mass spectrometer data. SUMS total pressure can be calculated by summing the individual species measurements as follows:

\[
P_t = k_s \sum \frac{I_i}{S_i}
\]

(1)

Figure 5a shows the results of the calculations from the data taken on STS-35 for the range valve closed condition using species \(N_2\), \(O_2\), \(CO_2\), \(Ar\), and \(NO\). Range valve closure occurs at 108 km, and the tubing system evacuation process is clearly observed in Fig. 5a. Included in Fig. 5a are the pressure transducer data over the same altitude interval. At these lower altitudes, pressure changes are rapidly transmitted through the tubing, but compositional changes are delayed. It would be expected, therefore, that the pressure transducer measurements are nearly instantaneous and that the lag between the mass spectrometer measurements and pressure transducer measurements represents the total lag of the mass spectrometer system. An apparent 0.2 km lag (1.5 s) is seen in Fig. 5a at the lower altitudes. Figure 5b shows the improved results, particularly below 95 km, after a 0.2 km upward altitude shift is applied to the SUMS data. This shift is based on the measured total pressure referenced to the start of the scan time. The individual ion currents have been interpolated to this common time.

**Leak Switch Transient**

The comparison between the pressure data and the mass spectrometer data at altitudes beyond the data transmission gap (above 97 km) does not compare well in Fig. 5b. The main difference is caused by the remnants of gas trapped in the tubing after the leak switch. Removing this transient requires an application of the pump-down characteristics of the system.

After the range valve closes, gas remains in the tubing and requires some time before it is pumped from the system. SUMS measures this gas in addition to the fresh gas that is sampled from the atmosphere. As a result, the data obtained after the range valve closes contains a decaying pressure transient, as shown in Fig. 6 for the nitrogen component. This transient pressure drop can be estimated by observing the system pump-down characteristics after the inlet valve closes, and no more external gas enters the system. By subtracting the percent drop per measurement time interval in the pump-down region, the transient can be removed from each of the species, and a corrected data set can be obtained. This correction can be applied to the data shown in Fig. 5b to obtain an improved measurement, particularly for altitudes above 95 km. When this effect is removed, excellent agreement is noted with the pressure transducer data, as shown in Fig. 7.

**Freestream Density Determination**

**Equilibrated Pressure Coefficient**

In flight, the total surface pressure measured at the SUMS inlet tube is higher than the freestream dynamic pressure. Inside the tube, the gas pressure quickly drops as it equilibrates to the wall temperature of the inlet tube. To obtain information about the ambient atmospheric conditions from the SUMS instrument, it is necessary to determine the relationship between the freestream pressure and the inlet tube equilibrated pressure, which is subsequently measured...
As continuum conditions are approached during re-entry, the flowfield coefficient ratio decreases, while the inlet coefficient ratio remains constant. This is because the flowfield coefficient ratio relates surface pressure to the equilibrated pressure, which is defined as

$$(C_p)_e = \frac{P_s}{\frac{1}{2} \rho V^2} = \frac{P_s}{q_\infty}$$

The $(C_p)_e$ values used in this analysis are shown as a function of $P_s$ in Fig. 8. The data from Ref. 8 are shown in the figure. Also shown in Fig. 8 is a curve derived from a combination of pressure and accelerometer flight data. The higher altitude $(C_p)_e$ data developed for the SUMS instrument did not extend to the lowest measurement altitudes. For this reason, an experimental pressure coefficient was developed based on pressures measured by the pressure transducers, accelerations measured by the high-resolution accelerometer package (HiRAP), and aerodynamic coefficients inferred from previous HiRAP flights. The experimental pressure coefficient is the product of a flowfield coefficient ratio that relates pressure to the freestream dynamic pressure and an inlet coefficient ratio that relates the equilibrated pressure to surface pressure. That is,

$$(C_p)_e = \frac{P_s}{q_\infty}$$

where $P_s$ is the pressure measured by the SUMS instrument. This equation is used to calculate the density from the pressure measurements.

Density Results
SUMS data were gathered from orbital altitudes (~346 km) down to approximately 87 km where the inlet valve closed. Figure 9 shows the altitude profile of the SUMS data. The density results are shown in Fig. 10. Table 1 shows the ratio of the SUMS measurements to the corresponding density obtained from the 1976 U.S. Standard Atmosphere model. The density values are compared to the reference model to determine if the SUMS data are consistent with the expected density profile. The table shows that the SUMS data are consistent with the 1976 U.S. Standard Atmosphere model at altitudes below 115 km, but above 115 km, the SUMS data show a decrease in density.

Density $\rho$ can be calculated from the pressure $P_s$ using the ideal gas law:

$$\rho = \frac{P_s}{RT}$$

where $R$ is the specific gas constant and $T$ is the temperature. The temperature is estimated from the flight data and is used to calculate the density. The density results are shown in Fig. 10. The density results are shown as a function of altitude in Fig. 10. The density values are compared to the 1976 U.S. Standard Atmosphere model. The density results are consistent with the model at altitudes below 115 km, but above 115 km, the SUMS data show a decrease in density.

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$$\rho = \frac{P_s}{RT}$$
System Background

The background levels of the spectra taken at orbital altitudes were extraordinarily high. An extensive investigation of the equipment after the flight revealed that ground composition air was trapped behind the filter within each pressure transducer connected in parallel to the mass spectrometer. Most of the trapped air escaped quickly when the Shuttle attained orbit. However, once in orbit, the pressure dropped, and free molecule flow conditions were reached causing the effective conductivity of the filters to drop to only a fraction of that at higher pressures. Under these conditions, the remaining air leaked continuously into the inlet tubing producing a small background pressure source while on orbit. The pressure was nearly constant at about 0.08 N/m², and the percent composition (N₂, O₂, Ar, and CO₂) matched sea-level air.

Figure 10 shows the effect of the trapped air background source on the density calculations. Above about 120 km, an exponential-like free-stream density decrease is expected, but the density is unreasonably high at a near constant level. Indeed, the density measurements eventually exceed a standard atmosphere by a factor of more than 10. A similar unreasonable density result occurs when the measurements are corrected by simply subtracting a constant background. Only by subtracting a semi-empirical variable background pressure can a reasonable behavior of density variation be obtained. Based on these results, it is concluded that the background pressure during the high-altitude measurements varies in a manner that requires further study of the conductance of the pressure filter before a reliable background model can be established. For this reason, the high-altitude data are not reliable. Below about 120 km, the pressure of the external gas rises high enough that the background source is no longer a contributing factor, and reliable results can be obtained. A background source pressure of 0.08 N/m² would lead to measurement errors of approximately 25, 7, and 1% at altitudes of approximately 120, 110, and 100 km, respectively. However, as the pressure in the tube rises, the conductance of the transducer filter that is trapping the gas changes, and at about 120 km, the apparent background pressure is less than 0.01 N/m², and errors are well within the 3% instrument error.

Fuel Dump Analysis

During a period of about 120 s, as the Orbiter descended through 320 km, pulses were observed in the SUMS spectra data for some of the species. Upon a closer examination of the HiRAP data on STS-35, it was clear that the spectra were affected by the ingestion of gas from the forward fuselage fuel dump of methylhydrazine (CH₃HN₂H₂). Figure 11a shows the Orbiter x body axis accelerometer data taken during re-entry. At about 18,300 s GMT, the HiRAP sensor detected a large (600 mg) x-axis disturbance that was traced to the forward fuselage fuel dump prior to the entry interface. An examination of the spectra data was made to determine if the fuel gas contaminants altered interpretation of the data at lower altitudes. Figure 11b shows the corresponding ion currents measured by SUMS for some selected species during the fuel dump time period. Most noticeable is the large peak at 15 amu/e⁻, which is assumed to be the methyl radical, CH₃. Both the methylhydrazine at 46 amu/e⁻ and HN₃H₂ (i.e., a free radical resulting from CH₃ splitting from methylhydrazine) at 31 amu/e⁻ show no appreciable increases and are not shown in Fig. 11b. Similarly, both the water at 18 amu/e⁻ and the OH at 17 amu/e⁻ show no peak.

The remaining species (N₂, O₂, CO₂, Ar, and O) all show increases in varying amounts. Nitrogen (28 amu/e⁻) shows a peak that could possibly be caused by a decomposition product of methylhydrazine or could be swept from the system walls. Ion peaks appear at 27 amu/e⁻ and the OH at 17 amu/e⁻ shows no peak. Similarly, both the water at 18 amu/e⁻ and the OH at 17 amu/e⁻ show no peak.

The 16-ion peak can be predicted using the ionization and cracking ratios in Table 1, assuming that the 16-ion peak was produced totally from O₂ (32) and CO₂ (44). When I₁₆ observed is divided by I₁₆ predicted using this assumption, a huge peak appears at the time of the dump as seen in Fig. 12b. The fact that this ratio is much larger than unity demonstrates that the 16 peak is not coming solely from O₂ and CO₂.

Figure 13 shows the ratio of I₁₄ measured to I₁₄ predicted, assuming I₁₄ predicted comes from doubly ionized N₂ and from doubly ionized CO, which comes from CO₂. The ratio is near unity throughout, except for a small drop at the time of the fuel dump, as can be seen in Fig. 13. This suggests that CO rises in the system slightly after the fuel dump over that produced from CO₂ fractionation, but is pumped from the system readily. Based upon the preceding analysis,
Chemistry Considerations

It is well known that high temperature flow phenomena at lower altitudes cause chemical reactions that change the local undisturbed atmospheric composition. Thus, it is expected that the composition measured by SUMS differs from the composition near the orifice entrance and is different from the ambient atmosphere. It is possible to gain some insights into the behavior of the gas composition near the Orbiter surface at the onset of aerodynamic heating. Mass spectrometer species data provide more information than a simple pressure transducer, but the information is not complete because the behavior of atomic oxygen (and other highly reactive species) is totally masked by a closed source system, such as SUMS.

The mole fraction, for species in a gas mixture containing species can be calculated using the equation,

\[ F_i = \sum_j \frac{P_i}{P_j}, \quad j = 1, 2, \ldots, n \]  

where \( P_i \) is the partial pressure of species \( i \), and the various \( P_j \) represent the partial pressures of the \( n \) gases measured by the mass spectrometer. The mole fractions for CO2, O2, and N2 are shown as a function of altitude in Fig. 14a. Together with Ar, which remains constant at approximately 1%, the partial pressures of these species combine to account for almost all of the pressure measured by the mass spectrometer on STS-35. For reference, Fig. 14b is a graph of the mole fractions of the ambient atmosphere based upon the 1976 U.S. Standard Atmosphere model. For these calculations, atomic oxygen is combined with O2 to represent the total number of oxygen molecules available to the mass spectrometer before flowfield chemistry. That is, all of the atomic oxygen that does not react with other elements, or is not adsorbed by the walls, combines to form O2 before it is measured by the mass spectrometer. As seen in Fig. 14a, the mole fractions remain fairly constant to about 100 km, similar to expectations without flowfield chemistry. At altitudes below about 100 km, the O2 and N2 mole fractions begin to decrease and the mole fraction of CO2 begins to increase. Because CO2 concentration rapidly increases, chemistry caused by aerodynamic heating has begun. There are at least two sources of carbon: one is the carbon in the steel tubing; and the other is the Orbiter's surface chin panel and nose cap, which are made of coated carbon–carbon materials. The exact method for the production of CO2 is not known, but a possible mechanism is that the heated carbon–carbon chin panels near the Orbiter's nose region interact with oxygen to produce a mixture of C, CO, and CO2. This mixture then reacts with atomic oxygen adsorbed to the walls of the inlet tubing and produces almost exclusively CO2 before being measured by the mass spectrometer. The possibility that some of the 44 amu peak was due to silicon monoxide, SiO, was considered, but, because of the extremely low vapor pressure of SiO at the tube temperature (about 12°C), extremely little gas would reach the mass spectrometer.

Source/Sink Estimates

The change in partial pressure of species \( i \), \( P_i \), caused by chemistry sources or sinks can be estimated using Eq. (4) by letting

\[ P'_i = P_i + \tau_i \]  

where \( P_i \) is the partial pressure of species \( i \), if there were no aerodynamic heating, and \( P'_i \) is the altered partial pressure of species \( i \) caused by aerodynamic heating (\( P'_i \) is measured by the mass spectrometer). The values of \( \tau_i \) can be solved by combining Eq. (5) with Eq. (4) and considering the mole fractions prior to aerodynamic heating as constants; that is, similar to Fig. 14b. Assuming that N2 undergoes no significant chemical changes due to initial heating results in four independent equations and four unknowns for a gas consisting of CO2, O2, and N2. The four unknowns are the pressures \( P_{CO2} \) and \( P_{O2} \) (both without chemistry changes), and the pressure changes \( \tau_{CO2} \) and \( \tau_{O2} \) at any altitude. The results from the solution of these equations, as a function of altitude, are shown in Fig. 15. The results, expressed as percentages, show that the production of CO2 is significant; over 20% of the gas measured at lower altitudes is CO2. Concurrently, at this altitude, oxygen is being depleted by about 7% of the total gas sampled, which represents nearly half of the oxygen measured.

It is worth reiterating that the actual chemical composition at the orifice entrance is probably different because of the presence of atomic oxygen. At altitudes near 100 km, the standard atmosphere model predicts an ambient composition containing about 10% atomic oxygen, O. Any molecular oxygen, O2, dissociation in the shock/boundary layer would produce additional atomic oxygen, but, as expected, atomic oxygen was not measured at any altitude during the SUMS experiment. This result suggests that O readily combined with carbon and other molecules before it was measured.
The SUMS experiment has provided partial pressure measurements in the altitude range from 180 to 87 km during STS-35 re-entry. However, above about 115 km altitude, the measurements are contaminated with sea-level composition air. The source of this contamination was identified as a slow release of gas trapped behind pressure transducer filters that were connected in parallel to the mass spectrometer. Below about 115 km, as the Orbiter surface pressure rises to values that are much larger than the trapped gas source, the sum of the SUMS partial pressure measurements correlate well with available local pressure transducer measurements. The freestream density in the rarefied-flow regime has also been calculated from available spectrometer. Below about 1 i 5 km, as the Orbiter surface pressure transducer filters that were connected in parallel to the mass spectrometer.}

**Acknowledgments**

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**References**