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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 to 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

- amu/e⁻ = atomic mass unit per unit charge
- \( (C_p)_{xe} \) = equilibrated pressure coefficient [see Eq. (2)]
- \( C_1, C_2 \) = inlet system flow restrictors (i.e., leaks)
- \( F_i \) = mole fraction of species \( i \)
- \( I_i \) = ion current of species \( i \)
- \( k_o \) = range valve constant; 140.0 for range valve closed or 1.0 for range valve open
- \( P_i \) = pressure of species \( i \), N/m²
- \( P_r \) = equilibrated pressure, N/m²
- \( P_s \) = surface pressure, N/m²
- \( P_t \) = total pressure due to all species, N/m²
- \( q_{\infty} \) = freestream dynamic pressure (i.e., \( (1/2) \rho V^2 \)), N/m²
- \( S_i \) = sensitivity coefficient of species \( i \), A/N/m²
- \( x, y, z \) = body axes
- \( V \) = velocity, m/s
- \( V_1, V_2, V_3 \) = inlet valve, dynamic range valve, and protection valve, respectively
- \( \alpha \) = angle of attack, deg
- \( \beta \) = sideslip angle, deg
- \( \rho \) = density, kg/m³
- \( \tau \) = change in pressure of species \( i \) due to chemical reactions, N/m²

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, 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 gas flows 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.
operation is controlled by stored Shuttle commands, and internal
the Shuttle computer and by internal "firmware" logic. The appli-
(VAMS) experiment that has been modified to provide mechanical,
the Viking (Mars mission) project upper atmosphere mass spectrometer
tape recorder and downloaded after the Shuttle flight.
more complete description of all of the components can be found
indicated a constant temperature of about 12°C during the flight. A
Fig. 3 Schematic of basic inlet system with approximate dimensions.

Fig. 4 Typical SUMS spectra taken on STS-35.

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 experi-
ment 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 spectrom-
eter 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 mea-
sured ion current in the mass spectrometer during flight. Currents
were also recorded for peaks that resulted from the double ioniza-
tion 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 CO2 disso-
icates and ionizes into CO+ and O+. Knowledge of the doubly
ionized to singly ionized current ratios and the cracking patterns al-
ows 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

<table>
<thead>
<tr>
<th>Gas</th>
<th>Mass, amu</th>
<th>Ion current ratios</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon monoxide, CO</td>
<td>28</td>
<td>1.12/1.28</td>
</tr>
<tr>
<td>Nitrogen, N2</td>
<td>28</td>
<td>1.14/1.28</td>
</tr>
<tr>
<td>Oxygen, O3</td>
<td>32</td>
<td>1.16/1.28</td>
</tr>
<tr>
<td>Argon, Ar</td>
<td>40</td>
<td>1.20/1.40</td>
</tr>
<tr>
<td>Carbon Dioxide, CO2</td>
<td>44</td>
<td>1.14/1.44</td>
</tr>
<tr>
<td></td>
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<td></td>
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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 tube. To obtain information about 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.

Fig. 5 SUMS total pressure and transducer measurements.

Fig. 6 SUMS nitrogen pressure measurements.

Fig. 7 Comparison of transducer data with SUMS total pressure measurements corrected for value closure transient and time lag.

Fig. 8 EQUIV. PRESSURE COEFFICIENTS.
The experimental pressure coefficient extends the DSMC analytic approach gradually to about 1.41, the modified Newtonian limit. The Moss and Bird data is used. In Fig. 8, the coefficient increases rapidly to reach the maximum value. Results of a seventh order curve fit to the flight data are shown for \( (C_p)^{1/2} \) in Fig. 8. This curve is used for pressures greater than 100 \( N/m^2 \). At lower pressures, a curve fit (not shown) to the Moss and Bird data is used. In Fig. 8, the coefficient increases steadily with pressure until reaching a value of about 1.5, from which it gradually declines to about 1.41, the modified Newtonian limit. The experimental pressure coefficient extends the DSMC analytic approach to higher pressures, but for pressures above 100 \( N/m^2 \), the experimental coefficient exceeds the theoretical limit of 1.41, which is calculated using the modified Newtonian approach for continuum hypersonic conditions. An explanation for this result is that when using any common criteria for continuum conditions, such as the ratio of molecular mean-free-path to characteristic length, the inlet coefficient reaches a continuum state before the flowfield coefficient.

A rearrangement of Eq. (2) can be applied to the SUMS equilibrated pressure measurements to allow the calculation of the dynamic pressure and, subsequently, the freestream density. That is, given \( P_e \) as measured by the SUMS (or a pressure transducer) and the \( (C_p)_e \) model (Fig. 8), the dynamic pressure is simply the ratio of these quantities. With dynamic pressure, the atmospheric density can be calculated because velocity is known from the trajectory reconstruction process.

### 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 as flown during a portion of the STS-35 reentry mission. SUMS spectra scans are transmitted continuously from de-orbit altitude, but, for this flight, the SUMS signal came out of the ground signal at about 180 km (labeled "Measurable Signal"). The delay in the signal emerging from the background signal was unexpected, and later investigations identified the cause to be trapped gas behind the filters of the pressure transducers. Details of the background signal are discussed later. Thus, during re-entry, SUMS data covered an interval of about 18 min from approximately 180 to 87 km. During this time interval, the Orbiter was at an angle-of-attack of about 45 deg, traveling at a speed of about 7500 m/s. Figure 9 also shows the altitude location of the range valve closure which switches leaks (labeled "Range Valve Closed") and allows measurements deeper into the atmosphere.

The density has been calculated from the mass spectrometer spectra using the method outlined in the previous section, and is shown in Fig. 10. Figure 10a shows a direct comparison with the density from the 1976 U.S. Standard Atmosphere model. Figure 10b shows the ratio of the SUMS measurements to the corresponding density obtained from the reference model; that is, the 1976 U.S. Standard. At altitudes less than 115 km, the SUMS data compare well with the model but exhibit density oscillations similar to those observed in accelerometry results from previous flights. Figure 10b shows an altitude wavelength of about 17 km that falls within earlier accelerometry measurements of between 15 to 40 km. At altitudes higher than 115 km, however, the data obviously are being influenced by the background gas.
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 as 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 freestream 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 conductances of the pressure filter before a reliable background level 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 × body axis accelerometer data taken during re-entry. At about 18,300 s GMT, the HiRAP sensor detected a large (600 µg) 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 (methy) radical, CH. Both the methylhydrazine at 46 amu/e⁻ and HN₂H₂ (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 both 32 and 16, but the 16 peak relative to its predump background readings is much larger than the 32 peak, compared to its background. If we examine the ratio I₆/I₃₂, shown on Fig. 12a, this difference becomes evident. Because the ratio persists at a level larger than the predump background and seems to decay toward it, this result suggests that CH₄ has been generated and is adhering to the walls. Below about 180 km, the ratio decreases abruptly as the O₂ concentration increases.

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 I₆/16 is divided by I₆/I₃₂ 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 I₆/I₄₄ measured to I₆/I₄₄ predicted, assuming I₆/I₄₄ 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,
For these calculations, atomic mass spectrometer on STS-35. For reference, Fig. 14b is a graph of 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 mass spectrometer species data provide more information than the spectra after the fuel dump showed that no significant permanent changes occurred due to the ingestion of the fuel gas into the system.

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 orbiter 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,

$$ F_i = \sum_j \frac{P_i}{P_j}, \quad j = 1, 2, \ldots, n \quad (4) $$

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 CO$_2$, O$_2$, and N$_2$ 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 O$_2$ 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 O$_2$ 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 O$_2$ and N$_2$ mole fractions begin to decrease and the mole fraction of CO$_2$ begins to increase. Because CO$_2$ 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 CO$_2$ 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 CO$_2$. This mixture then reacts with atomic oxygen adsorbed to the walls of the inlet tubing and produces almost exclusively CO$_2$ 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 $i$, $\tau_i$, caused by chemistry sources or sinks can be estimated using Eq. (4) by letting

$$ P'_i = P_i + \tau_i \quad (5) $$

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 $\tau$ 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 N$_2$ undergoes no significant chemical changes due to initial heating, results in four independent equations and four unknowns for a gas consisting of CO$_2$, O$_2$, and N$_2$. The four unknowns are the pressures $P$ (both without chemistry changes), and the pressure changes $\Delta P_{CO_2}$ and $\Delta P_{O_2}$ 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 CO$_2$ is significant; over 20% of the gas measured at lower altitudes is CO$_2$. 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 orbiter 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 10% atomic oxygen, O. Any molecular oxygen, O$_2$, 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.
Summary

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, 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 11 km, 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 the SUMS measurements. The procedure involved using an analytical/empirical model for the pressure coefficient at the SUMS orifice. The SUMS density measurements corroborate earlier accelerometer measurements that indicate density waves exist in the upper atmosphere relative to a Standard Atmosphere model with vertical wavelengths of 15–40 km. At 320 km, the SUMS registered the effects of the gas resulting from the Orbiter forward fuselage fuel dump. Examination of the spectra in this altitude region showed a large 15 amu ion current peak transient, probably CH₄, along with other species, but no significant permanent changes occurred because of the ingestion of the fuel gas into the system. The initial effects on gas composition because of aerodynamic heating were observed beginning at about 100 km. The production of CO₂ and the corresponding depletion of O₂ are clearly seen as the reactive gases from the flowfield, near the surface, react with the abundant carbon from the carbon–carbon nose and chin panels and, subsequently, with some of the atomic oxygen adhering to the tubing walls. It is estimated that at the lowest measurement altitude of SUMS (87 km), about 20% of the total pressure comes from CO₂.

Acknowledgments

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References