Trace Constituent Updates in the Marshall Engineering Thermosphere and Global Reference Atmospheric Model

C. G. Justus^a, Aleta Duvall^b, and Vernon W. Keller^c

Abstract

Global Reference Atmospheric Model (GRAM-99) is an engineering-level model of Earth's atmosphere. It provides both mean values and perturbations for density, temperature, pressure, and winds, as well as monthly- and geographically-varying trace constituent concentrations. From 0 km to 27 km, GRAM thermodynamics and winds are based on National Oceanic and Atmospheric Administration Global Upper Air Climatic Atlas (GUACA) climatology. Above 120 km, GRAM is based on the NASA Marshall Engineering Thermosphere (MET) model. In the intervening altitude region, GRAM is based on Middle Atmosphere Program (MAP) climatology that also forms the basis of the 1986 COSPAR International Reference Atmosphere (CIRA). Atmospheric composition is represented in GRAM by concentrations of both major and minor species. Above 120 km, MET provides concentration values for N₂, O₂, Ar, O, He, and H. Below 120 km, represented species also include H₂O, O₃, N₂O, CO, CH₄, and CO₂. At COSPAR 2002 a comparison was made between GRAM constituents below 120 km and those provided by Naval Research Laboratory (NRL) climatology. No current need to update GRAM constituent climatology in that height range was identified.

This report examines GRAM/MET constituents between 100 km and 1,000 km altitudes. Discrepancies are noted between GRAM/MET constituent number densities and mass density or molecular weight. Near 110 km altitude, there is up to about 25% discrepancy between MET number density and mass density (with mass density being valid and number densities requiring adjustment). Near 700 km altitude there is also up to about 25% discrepancy between MET number density and mean molecular weight (with molecular weight requiring adjustment). In neither case are MET mass density estimates invalidated. The discrepancies have been traced to MET subroutines SLV (which affects 90-170 km height range) and SLVH (which affects helium above 440 km altitude). With these discrepancies corrected, results are presented to illustrate GRAM/MET constituent mole fractions in terms of height-latitude cross sections from 100 km to 1,000 km altitude, and latitude-longitude "maps" at 450 km. Plans are discussed for an update of MET and GRAM to correct these constituent inconsistencies, and to incorporate several new thermospheric model features.

1. Introduction

At COSPAR 2002, results were presented (Justus et al., 2002) comparing trace constituent concentrations from NASA Marshall Space Flight Center's Global Reference Atmospheric Model, GRAM-99 (Justus et al., 1999) with those from a Naval Research Laboratory global

^aMorgan Research Corp.,ED44/Morgan, Marshall Space Flight Center, AL 35812, USA, jere.justus@msfc.nasa.gov

^bMorgan Research Corp.,ED44/Morgan, Marshall Space Flight Center, AL 35812, USA, aleta.duvall@msfc.nasa.gov

^cNASA Marshall Space Flight Center, ED44, Marshall Space Flight Center, AL 35812, USA, vernon.keller@nasa.gov

constituent climatology (Summers and Sawchuck, 1993). Based on results of that comparison, no evidence was found for a need to update GRAM constituent climatology in the low and middle atmosphere.

At thermospheric altitudes, GRAM is based on the Marshall Engineering Thermosphere or MET (Hickey, 1988; Owens et al., 1999), a modified version of the Jacchia (1970) thermosphere model. Although its primary application is to estimate thermospheric density variations, MET provides concentration values for molecular nitrogen (N₂), molecular and atomic oxygen (O₂ and O), argon (Ar), helium (He), and atomic hydrogen (H). The purpose of this paper is to examine thermospheric constituents from the MET-99 portion of GRAM-99, in the same way the COSPAR 2002 paper examined lower and middle atmospheric regions, to determine if there is a need to update or improve thermospheric constituent representations in GRAM.

MET-88 (Hickey, 1988) and MET-99 (Owens, 1999) are official model products of the Environments Group (ED44) at NASA Marshall Space Flight Center. It should be noted, however, that so-called MET Version 2.0 (Owens, 2002) is not an official MET release of the Marshall Environments Group, nor does it contain any updates or improvements beyond those in MET-99.

2. Problems with MET Number Densities and Mean Molecular Weight

Output from MET-99 includes exospheric temperature, local mass density (ρ) , temperature (T), pressure (P), number densities (Nd_i, i = 1,6) for the six MET constituents (N₂, O₂, O, Ar, He, and H), and mean molecular weight (M). If we denote individual constituent mole fractions by f_i, then number density is related to mass density by

$$Nd_i = f_i \rho N_{av}/M, \qquad (1)$$

where N_{av} is Avogadro's number. If we denote individual species molecular weights by M_i , then mean molecular weight is related to species molecular weights and number densities by

$$M = \sum (M_i Nd_i) / \sum Nd_i.$$
 (2)

In examining MET constituent output, it was noticed that there are internal discrepancies between mass density and number densities as implied by Eq. (1), or between mean molecular weight and number densities, as implied by Eq. (2). These errors are illustrated in Figure 1, which plots ratios of MET number density / correct number density, or MET mean molecular weight / correct molecular weight. Errors in number density of up to 25% are evident below 170 km altitude, while errors in mean molecular weight of up to 25% are seen above 440 km altitude.

Number density discrepancies illustrated in Figure 1 were traced to MET subroutine SLV, which computes seasonal-latitudinal variation in mass density below 170 km. This subroutine adjusted mass density for these effects, but did not adjust number densities to maintain the proper relationship of Eq. (1). This error can be corrected in MET by replacing original number densities with new values (Nd_i') below 170 km, where

$$Nd_i' = Nd_i N_{av} \rho / \Sigma (M_i Nd_i).$$
 (3)

Above 440 km, the error was traced to MET subroutine SLVH, which computes seasonal-latitudinal variations in hydrogen number density. This subroutine adjusted H number density, but did not adjust mean molecular weight to retain consistency required by Eq. (2). This error can be corrected by replacing original value of mean molecular weight with a new value (M') above 440 km, where

$$M' = \sum (M_i Nd_i) / \sum Nd_i.$$
 (4)

Note that mass density from MET did not require adjustment due to either of these two errors. Applying these corrections, we have used GRAM-99 to calculate constituent number density and mole fraction for various species. Example results are given in the following section.

3. Example Constituents from GRAM-99 Using Corrected MET-99

Figure 2 shows a height-latitude cross section of GRAM/MET-computed helium mole fraction for January at local solar time 13 hours. He mole fractions generally increase with increasing altitude, reaching values of 80% or larger by about 700 to 900 km. Minimum He mole fractions occur at latitudes slightly southward from the sub-solar point (about 22° S in January). For this time of day, maximum He mole fractions occur near the north pole. Figure 3 shows a latitude-time cross section of He mole fraction for January, at a height of 450 km. This figure shows minimum He mole fraction near 14 hours local solar time, with maximums at about the same latitude in the opposite hemisphere near 3 hours local solar time.

A height-latitude cross section of atomic hydrogen mole fraction for January, 13 hours local solar time is given in Figure 4. This figure shows a broad minimum for H mole fraction at low latitudes, with relative maximums in excess of 20% near both polar regions above about 850 to 950 km.

A molecular nitrogen latitude-time cross section at 450 km altitude is illustrated in Figure 5. In contrast to He mole fraction in Figure 3, N_2 mole fraction is at maximum near hour 14 at altitudes just south of the sub-solar point, with minimum near hour 3 at about the same latitude in the opposite hemisphere.

Figure 6 shows height-latitude cross section for atomic oxygen mole fraction (percent) for January at 13 hours local solar time. This figure shows O mole fraction having a relative maximum with altitude in excess of 90% between about 400 and 500 km. Figure 7 shows a latitude-time cross section for O mole fraction at 450 km, through this zone of near-maximum values. The pattern of maximum and minimum values of O mole fraction at this altitude is like that of N₂ in Figure 5, and opposite that of He mole fraction in Figure 3.

4. Conclusions

After correcting for above-mentioned inconsistencies in number densities or mean molecular weight, MET (as implemented in GRAM-99) produces reasonable patterns of altitude, latitude and time-of-day variation. Further studies should be conducted, comparing MET/GRAM constituents with those in other thermosphere models such as MSIS (Hedin, 1987; Picone et al., 2000, 2002), or with observed constituents (for example Bishop, 2001; Fennelly et al., 1993; Meier et al., 1992; Schoendorf and Oliver, 1998;).

Plans are underway to update MET, incorporating the corrections required by Eqs. (3) and (4), and to correct several other minor problems, not discussed in detail in this paper. Other minor problems in MET include use of a spherical Earth approximation instead of more realistic latitude variation of gravity and effective Earth radius, and small (≤ 1 %) discontinuities in density at year boundaries, day boundaries, and as a result of time resolution no finer than one minute. Other longer-term improvements planned for MET include updated semi-annual variations, such as those developed by Bowman (2004), and a number of other features requiring longer times for development and testing.

5. References

- Bishop, J. Thermospheric atomic hydrogen densities and fluxes from dayside Lyman alpha measurements. J. Atmos. Sol.-Terr. Phy. 63(4), 331-340, 2001.
- Bowman, B. R. The semiannual thermospheric density variation from 1970 to 2002 between 200-1100 km. Paper AAS 04-174 at American Astronautical Society 14th Space Flight Mechanics Meeting, Maui, Hawaii, February 8-12, 2004.
- Fennelly, J. A., Torr, D. G., Torr, M. R., Richards, P. G., Yung, Sopo. Retrieval of thermospheric atomic oxygen, nitrogen and temperature from the 732 nm emission measured by the ISO on ATLAS 1. Geophys. Res. Lett. 20(6), 527-530, 1993.
- Hedin, A. E. MSIS-86 Thermospheric Model. J. Geophys. Res. 92(A5), 4649-4662, 1987.
- Hickey, M. P. The NASA Marshall Engineering Thermosphere Model. Marshall Space Flight Center, NASA CR 179359, 1988.
- Jacchia, L. G. New Static Models of the Thermosphere and Exosphere with Empirical Temperature Profiles. Smithsonian Astrophysical Observatory, Special Report 313, 1970.
- Justus, C. G., Johnson, D. L. The NASA/MSFC Global Reference Atmospheric Model 1999 Version (GRAM-99). Marshall Space Flight Center, NASA/TM-1999-209630, 1999.
- Justus, C. G., Duvall, A. L., Johnson, D. L. Earth Global Reference Atmospheric Model (GRAM-99) and trace constituents, in press, Adv. Space Res., 2004.
- Meier, R. R., Feldman, U., Brown, C. M., Picone, J. M. Absolute O and O₂ concentrations in the thermosphere from Skylab occultation data. Planet. Space Sci. 40(8), 1153-1166, 1992.
- Owens, J. K., Niehuss, K. O., Vaughan, W. W., Shea, M. A. NASA Marshall Engineering Thermosphere Model 1999 Version (MET-99) and implications for satellite lifetime predictions. Adv. Space Res. 26(1), 157-162, 2000.
- Owens, J. K. NASA Marshall Engineering Thermosphere Model Version 2.0. Marshall Space Flight Center, NASA/TM-2002-211786, 2002.
- Picone, J. M., Hedin, A. E., Drob, D. P., Meier, R. R., Lean, J., Nicholas, A. C., Thonnard, S. E. Enhanced empirical models of the thermosphere. Phys. Chem. Earth, Pt. C 25(5), 537-542, 2000.
- Picone, J. M., Hedin, A. E., Drob, D. P., Aikin, A. C. NRLMSISE-00 empirical model of the atmosphere: statistical comparisons and scientific issues. J. Geophys. Res. 107(A12), 1468, doi:10.1029/2002JA009430, 2002.
- Schoendorf, J., Oliver, W. L. A comparison of thermospheric O derived at EISCAT with O predicted by MSIS. Geophys. Res. Lett. 25(12), 2119-2122, 1998.
- Summers, M. E., Sawchuck, W. Zonally Averaged Trace Constituent Climatology. A Combination of Observational Data Sets and 1-D and 2-D Chemical-Dynamical Model Results. Naval Research Laboratory, NRL-MR-7416 (DRAFT); NRL/MR/7641-93-7416 (DRAFT), 1993.

Figure 1. Molecular weight ratio or number density ratio (MET/Correct) versus height

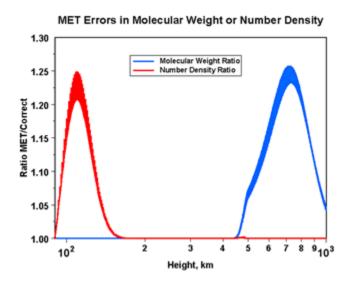


Figure 2. Height-latitude cross section of helium mole fraction (parts per million) for January at local solar time 13 hours

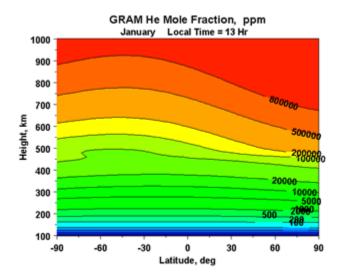


Figure 3. Latitude-time cross section of helium mole fraction (percent) for January at $450\,\mathrm{km}$ altitude

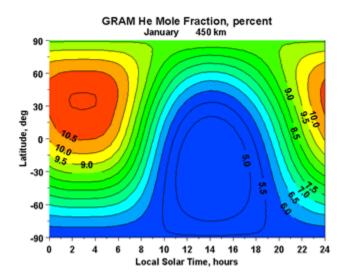


Figure 4. Height-latitude cross section of atomic hydrogen mole fraction (parts per million) for January at local solar time 13 hours

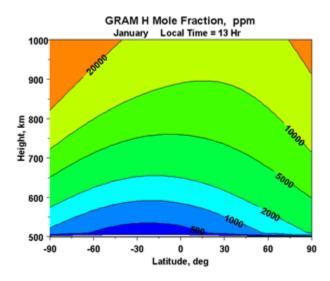


Figure 5. Latitude-time cross section of molecular nitrogen mole fraction (percent) for January at 450 km altitude

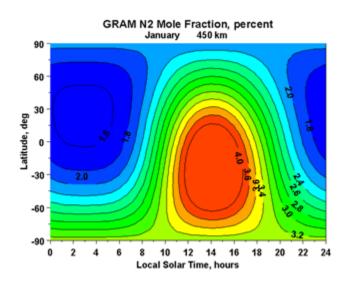


Figure 6. Height-latitude cross section of atomic oxygen mole fraction (parts per million) for January at local solar time 13 hours

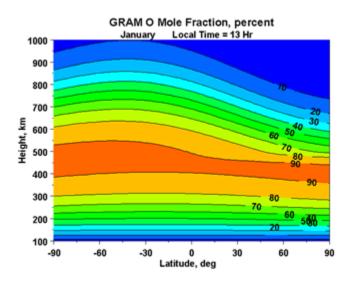


Figure 7. Latitude-time cross section of atomic oxygen mole fraction (percent) for January at 450 km altitude

