Vertical transport cycling and climatology of MLT constituent (e.g. O_x, H_x,CO_x, HO_x) distributions, 80-150 km

Gary Swenson, Fabio Vargas, and Pete Dragic, U of Illinois

September 2020

The climatology of minor species in the 80-150 km is important to the thermodynamics of the region, especially carbon dioxide and methane, which have large cooling effects on the region. Atomic oxygen, HOx, and COx, all participate in a cycling process, which can only be understood (modeled), only as well as the chemistry and vertical diffusion transport.

Constituents in the MLT, diffusively transport as molecular compounds from a chemically active region below 100 km, upward, to a photo-dissociation region. There, dissociation takes place, where simpler molecules and atoms are formed, which diffuse downward completing the cycle. The measured quantities to characterize and model the processes are the constituent distributions and vertical transport velocities. Measurements include classical passive methods coupled with Doppler LIDAR.

The morphology of the transport is the weakest, and least understood link in the process. Atomic oxygen is a key participant in the compounds, a participant in all the compounds. It is through the combined measurements of the constituent distributions and diffusive transport, that the constituent distributions and cycles, can be understood.

1 Identify essential science investigations necessary for major advancements in solar and space physics.

Atomic oxygen, a dominant constituent in the thermosphere, is diffusively coupled to it's reservoir in the mesosphere (80-105 km). Production varies with solar cycle, with season in a given hemisphere, and with seasons where gravity wave sources and wave filters vary, propagating from below. Atomic oxygen density, at any point in time, is most critical to the chemistry and role in forming molecular compounds including CO and CO_2, critical to the thermodynamics of the region.

The airglow observations of OH (night, 80-97 km) made by SABER [8, 6], analysis of CO and CO_2 profiles from SABER [9], and the 12 years of Envisat SCIAMACHY [11] measurements of OH and $O(^1S)$ by SCIAMACHY provided mean O density describe global mean k_{zz} profiles from 80-105 km, based on well established recombination chemistry, initially described by [1], and modified by [10].

Global average intra-annual variation (2x) in O density has been modeled with assumptions of variation in eddy transport (k_{zz}), a paramaterized method of turbulent transport, and a near constant O density in the mesosphere [7]. Intra-annual and hemispherical variation in the O density in the MLT is predictable, given the asynchronous nature of the production and loss of O. The O dissociation varies with solar inclination (season) and the eddy flux from below varies with orography, especially mountainous regions, as well as by dynamic filtering and ducting below 80 km. The hemispherical differences in O density are expected to be significant. The TIMED SABER instrument has measured O densities in the MLT region for 17+ years, with significant, intra-annual AO and SAO [work in progress, Vargas, et. al]. There are significant changes in the transport velocity with altitude in the 80-115 km, with traditional GW breaking effects below 97 km, and shear from tides (97-115 km) [5], above. What is the global and the intra-annual variability of these two, seemingly separately forced turbulent regions? The global mean k_{zz} is largest above 97 km [10].

Without the details of temporal/spatial (80-115 km) distribution of k_{zz}, one can't predict or model, the O density, nor it's chemical products, with the precision required.

2 Use the desired investigations to identify the research and capability development needed to meet the requirements of these missions.

Modeling of the atmospheric transport with the physics of the chemistry and dynamical processes are critical, such as found in the TIMED-GCM and WACCMX models. A mechanistic chemical model study by [3] was a state of understanding describing the minor density profiles of the atomic and molecular compounds in the MLT, where bi-direction transport is paramount to the process, such as downward diffusive transport of O and the return flux (upward) of O_2.

Composition and dynamic measurements are necessary, globally, from 80-150 km, for such a study. TIMED-SABER has measured most constituents 80-110 km. Wind measurements, such as those measured by ICON, from 90-150 km daytime, and 90-110 km at night. Ideally, composition and winds, globally, from 80-150 km, and turbulence from 80-115 km is crucial for the cycling study described herein. Constituent models define a few constituents, such as H_2, which are difficult to measure.

Certainly, event measurements such as those from a series of rocket and ground measurements can play a significant role, and should be continued to support the understanding of physical processes in the MLT. Diffusion times, however, are several weeks to a month, so averages over that time from are necessary, requiring satellite platforms to measure intra-annual and long term variabilities. Advection processes associated with waves and oscillations necessitate seasonal sampling over several years. Long term trends necessitate many 10's of years. Atomic oxygen may, for example, continue to decrease over a prolonged solar minimum period. O chemical recombination loss can continue with near constant eddy fluxes and downward transport, but production via dissociation is minimal.

3 Recognize research needed in the next decade to prepare for the long-term research goals.

Models: Add the sophistication of loss chemistry and bi-directional constituent transport to a MLT dynamic models.

Measurements: Composition and temperature, 80-150 km, 1 km resolution below 115 km, 3 km above, including O, CO, CO_2, HO_x, N_2, O_2, T. Measure turbulence and breaking GWs, and/or their effects, 80-115 km.

4 Recognize work needed to ensure a pipeline from basic research to pre-application research and then into operational needs, including the operations-to-research loop that strengthens forecasting and other predictive capabilities.

Models: Add the sophistication of loss chemistry and bi-directional constituent transport to the MLT dynamic models.

Measurements: Repeat the SABER instrument to continue the climatology of MLT T and constituents. Explore methods including LIDAR to cover 80-150 km O densities, day and night, incorporating methods developed by ground based Na lidar [4, 2]. 135.6 nm O density (and Doppler T) profiles using LIDAR from LEO is possible, but requires a laser power of 10 mW-1 W. Average powers of 10's of $/mu$Ws are readily achievable with today's semi-conductor technologies, but higher powers combined with 1-4 m^2 aperture receivers are required for the altitude range, especially to the MLT altitudes from a LEO orbiter. Fielding LIDAR on ISS or a similar platform where the required electrical power of $\geq$0.5 kW is available. Technological studies are required to implement the laser process as well as to develop optical efficiencies in those processes.

References

[1] F. D. Colegrove, F. S. Johnson, and W. B. Hanson. Atmospheric composition in the lower thermosphere. *Journal of Geophysical Research*, 71(9):2227–2236, 1966.

[2] Chester S. Gardner. Role of wave-induced diffusion and energy flux in the vertical transport of atmospheric constituents in the mesopause region. *Journal of Geophysical Research: Atmospheres*, 123(12):6581–6604, 2018.

[3] M. Grygalashvyly, E. Becker, and G. R. Sonnemann. Gravity wave mixing and effective diffusivity for minor chemical constituents in the mesosphere/lower thermosphere. *Space Science Reviews*, 168(1):333–362, 2012.

[4] Y. Guo, A. Z. Liu, and C.S. Gardner. First Na lidar measurements of turbulence heat flux, thermal diffusivity, and energy dissipation rate in the mesopause region. *Geophysical Research Letters*, 44:5782–5790, 2017.

[5] M. F. Larsen. Winds and shears in the mesosphere and lower thermosphere: Results from four decades of chemical release wind measurements. *Journal of Geophysical Research: Space Physics*, 107(A8):SIA 28–1–SIA 28–14, 2002.

[6] Martin G. Mlynczak, Linda A. Hunt, Jeffrey C. Mast, B. Thomas Marshall, James M. Russell, Anne K. Smith, David E. Siskind, Jeng-Hwa Yee, Christopher J. Mertens, F. Javier Martin-Torres, and et al. Atomic oxygen in the mesosphere and lower thermosphere derived from SABER: Algorithm theoretical basis and measurement uncertainty. *Journal of Geophysical Research: Atmospheres*, 118(11):5724–5735, 2013.

[7] Liying Qian, Stanley C. Solomon, and Timothy J. Kane. Seasonal variation of thermospheric density and composition. *Journal of Geophysical Research: Space Physics*, 114(A1), 2009.

[8] James M. Russell, Martin G. Mlynczak, Larry L. Gordley, Joseph J. Tansock, and Roy W. Esplin. Overview of the SABER experiment and preliminary calibration results. *Proc. SPIE 3756, Optical Spectroscopic Techniques and Instrumentation for Atmospheric and Space Research III*, 1999.

[9] Cornelius Csar Jude H. Salinas, Loren C. Chang, Mao-Chang Liang, Jia Yue, James Russell, and Martin Mlynczak. Impacts of SABER CO_2-based eddy diffusion coefficients in the lower thermosphere on the ionosphere/thermosphere. *Journal of Geophysical Research: Space Physics*, 121(12):12,080–12,092, 2016.

[10] G. R. Swenson, C. C. J. H. Salinas, F. Vargas, Y. Zhu, M. Kaufmann, M. Jones Jr., D. P. Drob, A. Liu, J. Yue, and J. H. Yee. Determination of global mean eddy diffusive transport in the mesosphere and lower thermosphere from atomic oxygen and carbon dioxide climatologies. *Journal of Geophysical Research: Atmospheres*, 124(23):13519–13533, 2019.

[11] Yajun Zhu and Martin Kaufmann. Atomic oxygen abundance retrieved from SCIAMACHY hydroxyl nightglow measurements. *Geophysical Research Letters*, 45(17):9314–9322, 2018.