Wave-induced transport of chemically active species in the mesosphere and lower thermosphere

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Wave-induced transport in the atmosphere is important to a wide range of research problems, including general circulation modelling, atmospheric chemistry modelling and thermal balance calculations. However, computational cost constraints mean that it is not practical to include small-scale wave transport effects directly in global models. The goal of this project is to bridge the gap between high-resolution regional models and global climate models in representing wave transport. It will contribute to a deeper understanding of the key wave-induced transport processes (advection, turbulent mixing, dynamical transport and chemical transport), their global characteristics and their impact on atmospheric chemistry. By developing a formalism – based on a new mathematical framework developed by Professor Chester Gardner at the University of Illinois [*Gardner*, 2018], who is a project partner - for incorporating these transport processes into global atmospheric chemistry models, this project will significantly enhance our ability to model the global constituent structure of the mesosphere and lower thermosphere (MLT) between 70 and 120 km. This region is sensitive to perturbations from below (upward propagating atmospheric waves and dynamical forcing) and above (solar radiation and energetic particle precipitation i.e. space weather), and is where interplanetary dust particles ablate. The MLT is also sensitive to longer-term climate change caused by stratospheric ozone depletion and increasing greenhouse gases [*Plane et al.*, 2015].

Tides, planetary waves and gravity waves play major roles in establishing the thermal structure and general circulation of the MLT. For example, the summer mesopause region is the coldest place in the atmosphere due to the meridional circulation induced by gravity wave (GW) dissipation. Less well known and understood are the equally important roles that waves play in vertical constituent transport, which is a fundamental atmospheric process that has profound effects on the chemistry and composition of the atmosphere below the turbopause. For example, atomic oxygen (O) is produced in the thermosphere above 120 km where photo-dissociation of O_2 is at a maximum. Dynamical processes, including molecular diffusion and wave effects, transport O downward into the upper mesosphere, where it is chemically depleted below 95 km, primarily through a series of exothermic reactions leading to the formation of mesospheric O_3 and the OH airglow layer (OH*). As such, O transport represents a transfer of chemical potential energy from the thermosphere to the mesosphere, and O is central to the chemistry and radiative balance of the MLT. The O, O_3, OH and HO_2 profiles, as well as the brightness of concomitant airglow emissions, are related to the speed of O transport, with faster transport corresponding to higher densities and brighter airglow. However, even though the chemistry of O and O_3 is well understood, global models – including NCAR's Whole Atmosphere Community Climate Model (WACCM) - significantly underestimate the observed mesospheric densities of these species (see Fig. 1), because the modelled downward transport from the thermosphere appears to be too slow [*Smith et al.*, 2015]**.** Waves, and the turbulence they generate, contribute to vertical constituent transport by inducing large-scale advection (upward in summer, downward in winter), eddy transport through turbulent mixing, dynamical transport associated with dissipating, non-breaking waves and chemical transport associated with perturbed chemistry [*Gardner and Liu*, 2016]. State-of-the-art global chemistry-climate models cannot resolve the ubiquitous small-scale waves and turbulence which permeate the upper atmosphere, and so generally focus on large-scale advection and eddy transport. For example, the standard version of WACCM with a horizontal grid of 1.9˚ latitude × 2.5˚ longitude has a horizontal resolution of ~200-300 km. However, it has been shown that wave-induced dynamical and chemical transport processes also play important roles: there is strong coupling of chemistry and temperature through reaction rates, giving rise to an additional turbulence-induced chemical vertical flux of mesospheric species such as O_3, O and Na. In addition, dissipating waves impart a downward velocity to constituents that is proportional to the heat transport velocity, a process termed dynamical transport to distinguish it from eddy and chemical transport. All these mechanisms induce significant constituent transport in the upper atmosphere, yet these dynamical and chemical transport processes driven by *sub-grid* waves have not been incorporated into any global atmospheric models.

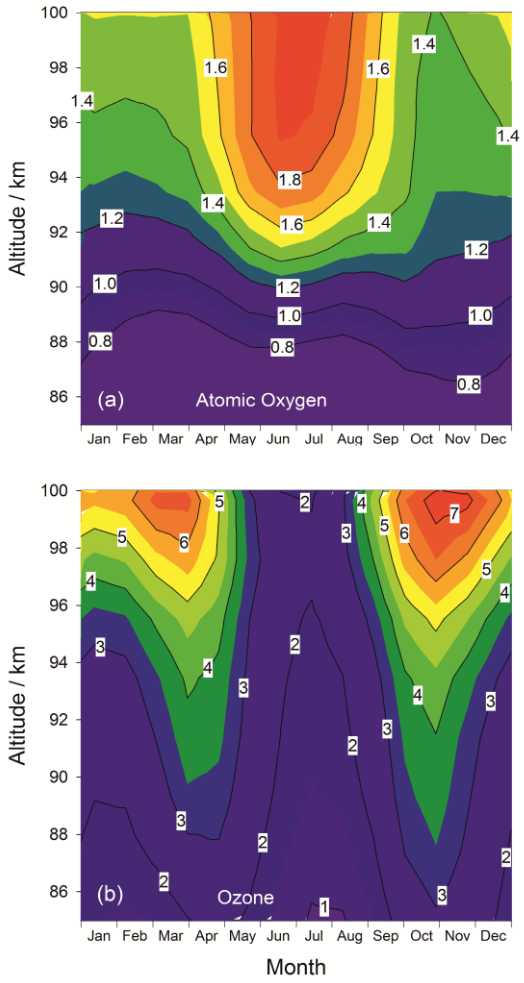

Figure 1. Measured/modelled ratio of the night-time concentration of a) O and b) O_3, as a function of height and month. Conditions: 35N, averaged from 2011-2014. Measurements from the SABER satellite instrument, model data from WACCM.

Objectives:

The overall goal is to enhance our understanding of wave transport processes and their relationships to chemistry by improving our ability to model the constituent structure of the MLT. The specific science goals are:

1) Assess how well a chemistry-climate whole atmosphere model (WACCM) characterizes vertical transport when run over a local region at sufficiently high horizontal resolution to resolve most of the GW spectrum.

2) Quantify the wave- and turbulence-induced vertical fluxes of Na, O, O_3 and HO_X in the MLT and determine their relationships to GW sources in the troposphere and stratosphere.

3) Determine the relative importance of vertical and horizontal transport in establishing the global distribution of these species and their seasonal variations.

4) Quantify the meteoric influx of Na with greater accuracy and hence resolve the total mass input of extra-terrestrial material into the Earth's atmosphere, thereby constraining astronomical models of dust evolution in the solar system, and better understanding the impacts of this dust throughout the atmosphere.

To achieve these goals we will:

1) Develop and use a regionally-refined (RR) version of WACCM to evaluate the impacts of resolving a portion of the currently unresolved GW spectrum on MLT constituents. Figure 2 illustrates a very high resolution WACCM run showing gravity waves evolving as a function of height, from a source east of Australia. The RR version is much more computationally efficient because only a region of the model is run at very high resolution.
2) Implement, test and validate a parameterization of the wave-induced dynamical and chemical transport processes for these key MLT constituents, in terms of the wave field statistics.
3) Incorporate these parameterizations into a new version of WACCM
4) Validate the upgraded WACCM against a range of satellite and lidar measurements and then use it to study the impact of wave transport on the global distribution and seasonal variations of the important, chemically active species Na, Fe, O, O_3 and HO_X.

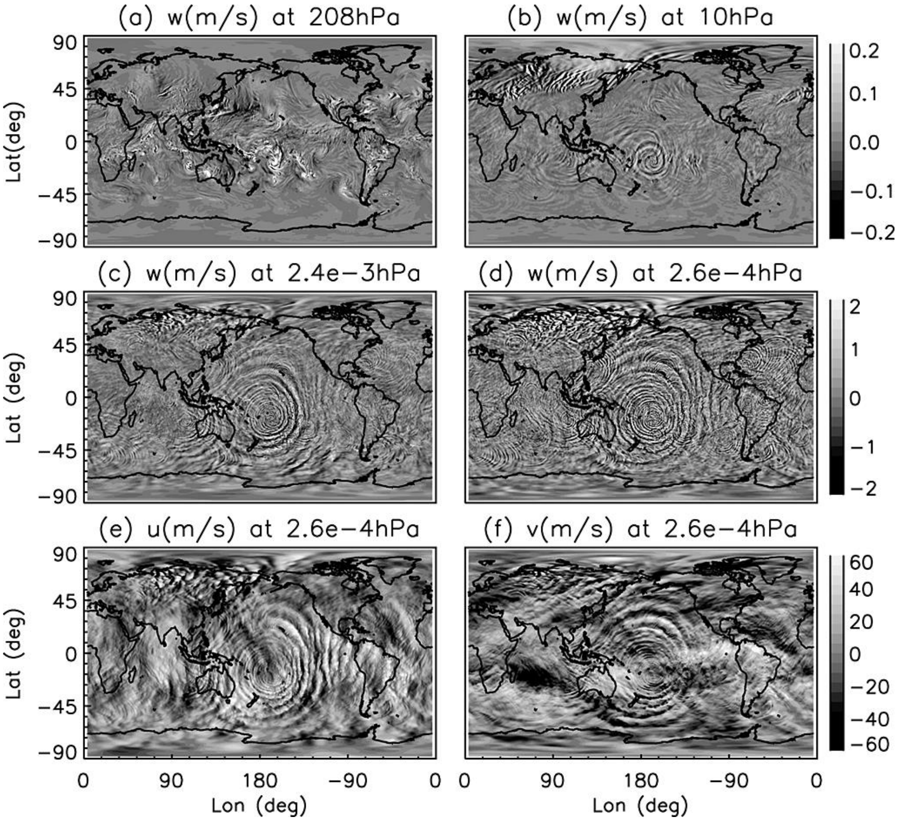

Figure 2.WACCM simulation with 0.25° × 0.25° horizontal resolution. Results on 4 February at 21:00 UT. (a–d) Vertical winds at 208 hPa (~11 km), 10 hPa (~30 km), 2.4 $\times 10^{-3}$ hPa (~87 km), and 2.6 $\times 10^{-4}$ hPa (~100 km), respectively. (e-f) Zonal and meridional winds at 2.6 $\times 10^{-4}$ hPa.

Potential for high impact outcome:

This project addresses wave-induced transport between regions of the atmosphere and the geospace environment. The parametrizations of wave-driven transport to be developed in the project will be generally applicable in any 3-D global model that uses a spectral model to parametrize gravity waves – in itself a major advance. The results will also be important for resolving a number of significant problems in the aeronomy of the MLT: the deficit of modelled O_3 and O compared to observations; the so-called HO_x dilemma, where the ratio of HO_2 to OH cannot be modelled correctly in both the stratosphere and mesosphere; the challenge of modelling the increase of CO_2 above 80 km; and modelling the measured fluxes of Na and Fe, and hence the cosmic dust input to the atmosphere. The project is therefore likely to have significant impacts in a number of fields, including global atmospheric modelling, aeronomy, solar system astronomy and atmospheric remote sensing.

Training:

The student will work under the supervision of Professor John Plane, Professor Daniel Marsh and Dr Wuhu Feng at the University of Leeds. Prof. Marsh also works at the world-leading US National Center for Atmospheric Research in Boulder, CO, and the student will have the opportunity to make an extended research visit to NCAR. This project will provide a high level of specialist scientific training in: (i) the application and development of a world-leading atmospheric chemistry-climate model; (ii) analysis and synthesis of large datasets; (iii) use of advanced High Performance Computing facilities. The student will also benefit from training organised by the Doctoral Training Programme, the National Centre for Atmospheric Science, and attendance at national/international conferences.

Further Reading:

Plane, J.M.C., W. Feng and E. Dawkins (2015), The Mesosphere and Metals: Chemistry and Changes, *Chem. Rev*., doi:10.1021/cr500501m.

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