Composition changes during disturbed conditions: Are mass spectrometers overestimating the concentrations of atomic oxygen?

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[1] Mass spectrometer measurements during disturbed conditions have shown that heavier gases like N₂ and Ar can be substantially enhanced while lighter gases like He can suffer moderate to severe depletions. Quantifying the changes in atomic and molecular oxygen is usually much more difficult as most mass spectrometers are not able to distinguish between ambient molecular oxygen and the molecular oxygen created by atomic oxygen-satellite surface reactions, but the paucity of molecular oxygen above 250 km normally allows one to attribute any molecular oxygen above 250 km to the recombination of atomic oxygen on a satellite surface. High resolution simulations presented in this study suggest that large amounts of molecular oxygen can be transported upwards by vertical winds during geomagnetic storms and that the neglect of this effect during geomagnetic storms has been studied intensively since the

[2] The response of the high latitude thermosphere to geomagnetic storms has been studied intensively since the 1950s and is now believed to be fairly well understood. The increased particle precipitation and electric fields cause Joule heating rates in the auroral regions to increase, generating large vertical winds [Rees et al., 1984] that can transport significant amounts of molecular nitrogen and oxygen upwards [Hays et al., 1973; Rishbeth et al., 1987]. These increased heating rates also alter the meridional pressure gradient, producing wind surges that propagate equatorwards [Forbes, 1989; Buonsanto et al., 1990]. The molecular species rich air that has been advected upwards is normally swept equatorwards by these meridional wind surges, with the early morning disturbances propagating furthest [Prolss, 1981]. Enhanced temperatures, nitric oxide densities and gravity wave generation are also observed in the auroral regions, with the largest-scale gravity waves propagating globally.

[3] While this picture is representative of a ‘typical’ storm, individual storms may not exhibit all of these characteristics as solar cycle variations, seasonal effects, storm strength and the time of the storm onset can all affect the evolution of these disturbances. Despite this variability, simulations by general circulation models [Burns et al., 1991; Fuller-Rowell et al., 1994, 1996] and two-dimensional models [Skoblin and Förster, 1995] have been able to reproduce most of the salient features of these disturbances, providing valuable insights into their development and evolution. However, these models have not been able to reproduce the large vertical winds frequently observed at higher latitudes as they do not solve the vertical momentum equation self-consistently.

[4] The presence of these vertical winds will complicate the interpretation of mass spectrometer measurements at higher latitudes as most mass spectrometers are not able to distinguish between atomic and molecular oxygen. This fact was normally not an issue at higher altitudes as the paucity of molecular oxygen at these heights usually allowed one to attribute any measured molecular oxygen to the recombination of atomic oxygen on a satellite surface. The vertical transport of molecular nitrogen and oxygen by large vertical winds to higher altitudes invalidates this assumption, which means that only mass spectrometers with the ability to differentiate between ambient molecular oxygen and the molecular oxygen created by atomic oxygen-satellite surface reactions will be reliable under these conditions. This fact is frequently overlooked in the literature and will be investigated more thoroughly in this paper as the composition changes inferred from mass spectrometer measurements have played an important role in our understanding of the disturbed upper atmosphere.

2. Model Description

[5] The model used in this study is based on one previously developed by Chang and St.-Maurice [1991]. It solves the mass, momentum, and energy equations for a viscous, thermally conducting, multicomponent gas in a zonally symmetric, spherical coordinate system using the method of MacCormack [1969]. The initial temperature and number density profiles used in the neutral component of the model have been determined from a self-consistent, latitudinally invariant calculation and are very similar to the predictions of MSIS90e [Hedin, 1991] at high latitudes during geomagnetically quiet, solar minimum, daytime conditions. The ion density profile is latitudinally invariant and corresponds to the ‘strongly disturbed’ ionization pro-
file employed by Chang and St.-Maurice [1991], which had a peak E-region density of $10^6$ cm$^{-3}$ and an essentially constant number density of $10^6$ cm$^{-3}$ above 225 km. The composition percentages of the ionospheric species are also typical for strongly disturbed conditions, with the NO$^-$, O$_2^-$, and O$^+$ percentages corresponding to the predictions of a TRANSCAR simulation with a 100 mV/m electric field [Blelly et al., 1996]. These ‘strongly disturbed’ ionospheric conditions were used for the entire simulation as the ionospheric component of the model is currently time-independent (a coupled thermosphere-ionosphere version of the model is being developed).

The evolution of the geomagnetic disturbance in this simulation is controlled by the location, magnitude, and width of the imposed electric field, which was approximated by a Gaussian function of 0.5° half-width on the geomagnetic field line that emerges from the Earth’s surface at 70°N. It was always directed equatorially and increased linearly in strength from 0 mV/m to 100 mV/m during the first 1000 seconds of the simulation. Once the electric field attained its maximum value, it was maintained at this value for the remainder of the simulation to ensure that steady-state values were achieved. Simulations where the electric field was turned off in the latter part of the simulation have vertical winds that eventually decay to zero.

The large vertical winds that are being generated in this simulation will transport significant amounts of molecular nitrogen and molecular oxygen upwards. Plots of R(n) (the ratio of the disturbed number density to its quiet-time “background” value) at an altitude of 280 km are plotted in the upper panel of Figure 3 for N$_2$ (blue), O$_2$ (red), and O (green) at 70°N. The number densities of N$_2$, O$_2$, and O are all increasing during the first 20 minutes of the simulation as Joule heating is causing the auroral zone to expand (this can also be seen in the neutral density ratios). The next 30 minutes are dominated by vertical transport effects, with the N$_2$ and O$_2$ ratios continuing to increase. The N$_2$/O$_2$ rich air that is causing the N$_2$ and O$_2$ ratios to increase is also atomic oxygen poor, causing the atomic oxygen ratios to

3. Results and Discussion

As the electric field strength increases, the enhancements in Joule heating and Lorentz forcing will generate large zonal winds and a vertical-meridional wind system in the region of heating. A contour plot of the vertical winds obtained at the 30 minute mark of the simulation is presented in Figure 1 and shows that vertical winds with speeds in excess of 150 m/s are being generated in the auroral region. Vertical wind speeds of this magnitude are not that unusual and have been observed by ground-based Fabry-Perot interferometers (FPs) at high latitudes since the early 1980s (see the review by Smith [1998]).

Time series of the vertical wind speeds at 180 km, 240 km and 300 km at 70°N show that there are two stages in the evolution of the vertical winds: an acceleration phase that correlates with the increasing electric field strength and a steady state phase where the wind speeds approach an asymptotic value with weak oscillations superimposed on it (Figure 2). The vertical wind time series at 300 km reaches a maximum value of 166 m/s after 19 minutes of simulation time and then decreases to a near steady-state value of 70 m/s. The vertical winds at 180 km and 240 km also reach their maximum values of 78 m/s and 126 m/s after 19 minutes, but their asymptotic values are 75 m/s and 60 m/s, 5 m/s greater and 10 m/s slower than the value obtained at 300 km. Studies by Rees et al. [1984] and Sica et al. [1986] have noted very similar behaviour, with vertical winds exhibiting a sudden increase which is followed by oscillations that damp out over several hours. The vertical wind time series shown in Figure 2 approach a non-zero asymptotic value in the latter part of the simulation as the electric field has been left on at its maximum value; simulations where the electric field was turned off in the latter part of the simulation have vertical winds that eventually decay to zero.

The large vertical winds that are being generated in this simulation will transport significant amounts of molecular nitrogen and molecular oxygen upwards. Plots of R(n) (the ratio of the disturbed number density to its quiet-time “background” value) at an altitude of 280 km are plotted in the upper panel of Figure 3 for N$_2$ (blue), O$_2$ (red), and O (green) at 70°N. The number densities of N$_2$, O$_2$, and O are all increasing during the first 20 minutes of the simulation as Joule heating is causing the auroral zone to expand (this can also be seen in the neutral density ratios). The next 30 minutes are dominated by vertical transport effects, with the N$_2$ and O$_2$ ratios continuing to increase. The N$_2$/O$_2$ rich air that is causing the N$_2$ and O$_2$ ratios to increase is also atomic oxygen poor, causing the atomic oxygen ratios to

![Figure 1](image1.png)

**Figure 1.** Vertical winds at the 30 minute mark of the simulation. The vertical winds are confined to the region of Joule heating and reach a maximum value of 155 m/s at 330 km.

![Figure 2](image2.png)

**Figure 2.** Vertical wind time series at 70°N at 180 km (blue), 240 km (green) and 300 km (red). The vertical winds in the 300 km time series reach a maximum value of 166 m/s at the 19 minute mark of the simulation.
The simulated \( \text{O} + 2 \text{O}_2 \) of a geomagnetic storm on October 29, 1973 \([\text{Prölls}, 1980]\). The ratios of \( \text{N}_2 \) (blue), \( \text{O}_2 \) (red), \( \text{O} \) (green) and \( \rho \) (black) all increase during the first 20 minutes of the simulation, but the subsequent evolution of the individual species is controlled by meridional and vertical transport (see the text for more details). The \( \text{O} + 2 \text{O}_2 \) ratios (black) are much larger than the atomic oxygen ratios (green) in the region of heating at the 90 minute mark of the simulation as significant amounts of molecular oxygen have been transported upwards.

Meridional transport starts to become effective in the second hour of the simulation, which results in an eventual equilibrium between vertical and meridional transport, i.e. all of the number density ratios stabilize as the meridional winds are transporting the air equatorwards as quickly as the vertical winds can transport it upwards.

The ratios of \( \text{N}_2 \) (blue), \( \text{O}_2 \) (red), \( \text{O} \) (green) and \( \text{O} + 2 \text{O}_2 \) (black) have also been plotted as a function of latitude at the 90 minute mark of the simulation in the lower panel of Figure 3. The number densities of \( \text{N}_2 \) are 6.5 times greater in the region of heating and exhibit a steep latitudinal gradient, in good agreement with ESRO-4 observations of a geomagnetic storm on October 29, 1973 \([\text{Prölls}, 1980]\). The simulated \( \text{O} + 2 \text{O}_2 \) ratios are also consistent with the observed ESRO-4 atomic oxygen ratios for October 29, 1973, which may appear to be quite contradictory. However, ESRO-4 (like most other mass spectrometers) did not measure atomic oxygen directly; atomic oxygen number densities at higher altitudes were inferred from the expression \( \text{O} + 2 \text{O}_2 \) as any molecular oxygen measured at these altitudes was attributed to the recombination of atomic oxygen on a satellite surface. The ability of these simulations to separate the \( \text{O} + 2 \text{O}_2 \) ratio into atomic and molecular oxygen shows that the concentrations of molecular oxygen are not negligible at high latitudes during strongly disturbed conditions; the molecular oxygen number densities are 25 times greater in the region of heating while the atomic oxygen concentrations are actually one-seventh of their quiet-time values.

This apparent overestimation of atomic oxygen number densities by ESRO-4 means that the \( \text{N}_2/\text{O} \) ratios inferred from ESRO-4 could also be in error. Plots of the \( \text{N}_2/(\text{O} + 2 \text{O}_2) \) ratio at 280 km at the 30, 60, 90, and 120 minute marks of the simulation are presented in Figure 4 and approach a value of 15, in good agreement with ESRO-4 observations on October 29, 1973 \([\text{Prölls}, 1980]\). The actual \( \text{N}_2/\text{O} \) ratios may be much higher, with values of 45–55 being more realistic if the majority of the molecular oxygen being detected by ESRO-4 at these altitudes is due to vertical transport.

It should be emphasized that the transport of molecular oxygen to higher altitudes during disturbed conditions is not a new idea; it has been noted in previous numerical studies \([\text{e.g. Hays et al., 1973}]\), and has been observed experimentally by \textit{Potter et al.} [1979]. \textit{The Potter et al.} [1979] study demonstrated that the molecular nitrogen and molecular oxygen densities at 200 km were \( \sim 2.5 \) and \( \sim 4 \) times larger during a geomagnetic storm on January 10, 1976 by analyzing ‘fly-through’ mode data from the open source neutral mass spectrometer (OSS) on AE-D. The simulated \( \text{N}_2 \) and \( \text{O}_2 \) density increases at 200 km are larger than this, but a more moderately disturbed simulation is consistent with these changes (not shown).

While the amounts of molecular nitrogen and oxygen transported upwards are sensitive to the heating rates, the fact that significant amounts of molecular oxygen can be transported upwards with molecular nitrogen suggests that high latitude mass spectrometer measurements may need to be reexamined in light of these new results. Localized enhancements of molecular nitrogen are routinely observed in the polar cap region at all levels of geomagnetic activity \([\text{Hedin and Reber, 1972; Reber and Hedin, 1974; Taueusch and Hinton, 1975; Laux and von Zahn, 1979}]\) and, if they are accompanied by enhancements in molecular oxygen, then mass spectrometer observations of atomic oxygen in this region may be in significant error. The retrieval of

![Figure 3](image-url) Composition ratios at 280 km (top) as a function of time at 70°N and (bottom) as a function of latitude at the 90 minute mark of the simulation. The ratios of \( \text{N}_2 \) (blue), \( \text{O}_2 \) (red), \( \text{O} \) (green) and \( \rho \) (black) all increase during the first 20 minutes of the simulation, but the subsequent evolution of the individual species is controlled by meridional and vertical transport (see the text for more details). The \( \text{O} + 2 \text{O}_2 \) ratios (black) are much larger than the atomic oxygen ratios (green) in the region of heating at the 90 minute mark of the simulation as significant amounts of molecular oxygen have been transported upwards.

![Figure 4](image-url) \( \text{N}_2/\text{O} \) and \( \text{N}_2/(\text{O} + 2 \text{O}_2) \) ratios at 280 km. The ratios of \( \text{N}_2/\text{O} \) and \( \text{N}_2/(\text{O} + 2 \text{O}_2) \) with respect to their quiet-time values are plotted at the 30 minute (star), 60 minute (dash-dotted), 90 minute (dashed), and 120 minute (solid) marks of the simulation. The \( \text{N}_2/\text{O} \) ratios are much larger than the \( \text{N}_2/(\text{O} + 2 \text{O}_2) \) ratios in the second hour of the simulation.
atomic hydrogen densities from mass spectrometer measurements at high latitudes may also be in error as the number densities of atomic hydrogen are normally derived from atomic oxygen measurements (see Sanatani et al. [1995] and references therein for more details).

4. Conclusions

The high resolution simulations presented in this paper has shown that numerical models are now capable of reproducing the large vertical winds observed in the high latitude thermosphere. They have also shown that these vertical winds can transport significant amounts of molecular nitrogen and oxygen upwards, suggesting that many mass spectrometer measurements of atomic and molecular oxygen in the polar cap region and during strongly disturbed conditions may be in error. Current climatologies of the high latitude thermosphere and our understanding of how the thermosphere-ionosphere system responds to large inputs of energy should be reexamined in light of these new results.

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References


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