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2 **Vertical Transport of Sensible Heat and Meteoric Na by the Complete Temporal Spectrum**
3 **of Gravity Waves in the MLT Above McMurdo (77.84°S, 166.67°E), Antarctica**

4

5 Xinzhao Chu^{1*}, Chester S. Gardner^{2*}, Xianxin Li^{1,3}, and Cissi Ying-Tsen Lin^{1,4}

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7 ¹Cooperative Institute of Research in Environmental Sciences & Department of Aerospace
8 Engineering Sciences, University of Colorado Boulder, Boulder, CO 80309, USA

9 ²Department of Electrical and Computer Engineering, University of Illinois, Urbana, IL, USA

10 ³Institute of Oceanographic Instrumentation, Qilu University of Technology, Shandong
11 Academy of Sciences, Qingdao, China

12 ⁴Department of Space Science & Engineering, National Central University, Taiwan

13 *Corresponding authors: Xinzhao.Chu@colorado.edu and cgardner@illinois.edu

14 **Key Points:**

15 1) We report the first observations of vertical fluxes of sensible heat & Na induced by the
16 complete temporal spectrum of gravity waves

17 2) McMurdo sensible heat and Na fluxes exhibit large downward peaks near 84 km and
18 large upward sensible heat fluxes occur at ~97–106 km

19 3) Sensible heat & Na flux measurements support theories and show significant impacts of
20 wave-induced vertical transport and secondary waves

21 **Abstract**

22 We report the first lidar observations of vertical fluxes of sensible heat and meteoric Na
23 from 78–110 km in late May 2020 at McMurdo, Antarctica. The measurements include
24 contributions from the complete temporal spectrum of gravity waves and demonstrate that wave-
25 induced vertical transport associated with atmospheric mixing by non-breaking gravity waves,
26 Stokes drift imparted by the wave spectrum, and perturbed chemistry of reactive species, can

27 make significant contributions to constituent and heat transport in the mesosphere and lower
28 thermosphere (MLT). The measured sensible heat and Na fluxes exhibit downward peaks at 84
29 km (-3.0 Kms^{-1} and $-5.5 \times 10^4 \text{ cm}^{-2}\text{s}^{-1}$) that are ~ 4 km lower than the peak fluxes observed at
30 midlatitudes. This is likely caused by the strong downwelling over McMurdo in late May. The
31 Na flux magnitude is double the maximum at midlatitudes, which we believe is related to strong
32 persistent gravity waves in the MLT at McMurdo. To achieve good agreement between the
33 measured Na flux and theory, it was necessary to infer that a large fraction of gravity wave
34 energy was propagating downward, especially between 80 and 95 km where the Na flux and
35 wave dissipation were largest. These downward propagating waves are likely secondary waves
36 generated in-situ by the dissipation of primary waves that originate from lower altitudes. The
37 sensible heat flux transitions from downward below 90 km to upward from 97–106 km. The
38 observations are explained with the fully compressible solutions for polarization relations of
39 primary and secondary gravity waves with $\lambda_z > 10 \text{ km}$.

40 **Plain Language Summary**

41 The upper atmosphere is filled with waves that originate in the lower atmosphere from
42 storm systems and airflow over mountainous terrain, and then propagate upward. These waves
43 play key roles in establishing the composition and temperature structures by mixing the upper
44 atmosphere and by perturbing chemical reactions of important reactive species like atomic
45 oxygen and ozone. By using meteoric sodium (Na) that is injected between 78 and 110 km
46 altitude by the vaporization of cosmic dust, as a tracer, and exciting the Na atoms to fluorescence
47 using a lidar system located at McMurdo Station, Antarctica, we directly measured the vertical
48 transport of heat and Na induced by the full spectrum of waves. A surprising discovery is the
49 positive heat flux in the lower thermosphere (97–106 km), which contradicts conventional
50 thinking but demonstrates the importance of the fully compressible solutions for polarization
51 relations of primary and secondary gravity waves. By comparing the measured Na transport with
52 theory, we also show that many of the waves between 80 and 95 km are propagating downward,
53 which are likely generated in this region when upward propagating waves become unstable and
54 break, much like ocean waves behave when breaking over a shoal.

55 **1. Introduction**

56 The spectrum of atmospheric gravity waves drives the global circulation and controls the
57 vertical transport of heat and constituents in the mesosphere and lower thermosphere (MLT).
58 Dissipating waves exert a drag on the mean horizontal flow (Lindzen, 1981; Holton, 1982 &
59 1983), while both dissipating and non-dissipating waves, induce strong vertical mixing of the
60 atmosphere (Hickey et al., 2000; Gardner et al., 2019; Liu, 2021), alter molecular and eddy
61 diffusion by perturbing constituent mixing ratios (Grygalashvyly et al., 2012; Gardner, 2018),
62 and drive the chemical transport of reactive species by modulating their chemical reactions
63 (Walterscheid & Schubert, 1989; Gardner & Liu, 2010 & 2016). Non-breaking gravity waves
64 also induce a net heat flux (Walterscheid, 1981; Weinstock, 1983) in addition to the diffusive
65 heat transport caused by turbulence arising from breaking waves (Lindzen, 1981).

66 Wave-driven heat and constituent transport are characterized by the vertical fluxes of
67 sensible heat and constituents, which are defined as the expected values of the product of the
68 vertical wind fluctuations (w') times the temperature (T') and constituent density (ρ'_C)
69 fluctuations induced by the gravity wave spectrum. Observations of these important parameters
70 are rare because it is necessary to measure simultaneously, over long periods of time, the vertical
71 wind (w), temperature (T), and constituent number densities (ρ_C), to derive statistically
72 significant estimates of the fluxes. The first observations of sensible heat flux ($\overline{w'T'}$, overbar
73 denotes sample average) in the MLT were reported from Haleakala, HI (20.7°N) using a Na
74 Doppler lidar (Tao & Gardner, 1995) followed by more extensive observations at the Starfire
75 Optical Range, NM (SOR, 35°N) (Gardner & Yang, 1998). Na flux ($\overline{w'\rho'_{\text{Na}}}$) observations were
76 first reported from SOR (Liu & Gardner, 2004) and then from Haleakala (Liu & Gardner, 2005).
77 These observations have revealed that the heat and Na fluxes peak just below 90 km, with
78 maximum downward (negative) values of -1 to -3 Km/s and -1×10^4 to $-3 \times 10^4 \text{ cm}^{-2}\text{s}^{-1}$
79 (Gardner & Liu, 2007 & 2010). More significantly, the heat flux convergence induces strong
80 cooling near 90 km that can approach -50 Kd^{-1} for the annual mean (Gardner & Liu, 2007).
81 Furthermore, the large downward Na flux near 90 km is 5–10 times larger than the expected
82 eddy flux, which implies that the cosmic dust influx, the source of all the mesospheric metal
83 layers, is much larger than previously assumed (Carrillo-Sánchez et al., 2016). More recently, the
84 Fe and Na fluxes were measured simultaneously at Table Mountain, CO (40°N). These
85 observations have demonstrated that the cosmic dust particles responsible for injecting a large

fraction of the ablated material into the Earth's upper atmosphere enter at relatively slow speeds and originate primarily from the Jupiter Family of Comets (Huang et al., 2015; Carrillo-Sánchez et al., 2015, 2016). Long-term Na lidar observations of gravity wave momentum, heat and Na fluxes conducted at Hefei, China (32°N), exhibit smaller values for all three parameters (Tao Li, private communication, University of Science and Technology of China), which may reflect significant differences in wave activity at this site compared to SOR, Haleakala, and Table Mountain. Most recently, sensible heat and potential temperature fluxes ($\overline{w'\theta'}$, θ = potential temperature) have been reported from Cerro Pachón in the Chilean Andes (30°S), which are more in line with the profiles observed at SOR and Haleakala (Guo & Liu, 2021).

All these previous measurements of heat and constituent fluxes were made at mid-latitudes by employing nighttime data with observation periods less than about 8–10 h, which do not include the effects of inertial-period gravity waves. Here, we report the first lidar measurements of the vertical fluxes of meteoric Na and sensible heat at extremely high latitudes using vertical wind, temperature, and Na observations, made at McMurdo Station (77.84°S, 166.67°E) in May 2020. Because the inertial period at McMurdo is 12.3 h, and the two observation periods utilized for this study each exceeded 16 h, the derived fluxes represent contributions of the complete gravity wave temporal spectrum from the inertial frequency (f) to the buoyancy frequency (N).

In contrast to the previous reports of fluxes between 85 and 100 km at midlatitudes, the acquisition of high-quality lidar data at McMurdo (Chu et al., 2020) and application of an innovative data processing technique (Gardner & Chu, 2020) have enabled the extension of flux measurements into the lower thermosphere (100–110 km) and below 85 km to nearly 75 km. A surprising discovery is the positive (upward) sensible heat flux between 97–106 km, which contradicts the traditional understanding of wave-driven heat transport, but aligns well with the earlier findings of super-exponential growth of tidal and planetary wave amplitudes in temperature from 100 to 110 km (Fong et al., 2014, 2015; Lu et al., 2017a). We show that the positive heat fluxes are predicted by the fully compressible solutions for the polarization relations (Vadas, 2013) of upward-propagating, non-dissipative gravity waves. When the spectrum is dominated by energetic waves with mesoscale vertical wavelengths ($\lambda_z \sim 20 \text{ km}$), as is predicted by models (Vadas et al., 2018; Vadas and Becker, 2019) and is often observed in the

116 lower thermosphere (e.g., Chu, Yu, et al., 2011; Chen et al., 2016), the phase difference between
117 w' and T' is about $8^\circ - 9^\circ$ less than 90° , and consequently, the positive heat flux is expected to
118 approach several $+Kms^{-1}$. The presence of external heat sources and/or wave amplification in
119 the lower thermosphere over McMurdo may also contribute to the positive heat flux, possibly via
120 introducing additional phase shift between w' and T' by energy input and forcing from the
121 magnetosphere and ion-neutral coupling or via wave amplification caused by large wind shears
122 and instabilities. The McMurdo flux profiles are compared to those previously observed at
123 several mid-latitude sites and show that wave-driven atmospheric mixing plays a significant role
124 in establishing the thermal and constituent structures of the polar upper atmosphere. In particular,
125 the comparison of the measured Na flux profile with theory demonstrates the importance of
126 vertical Stokes drift induced by the full wave spectrum, chemical transport for chemically active
127 species like Na, and the influence of downward-propagating waves, especially in regions of
128 strong wave dissipation. The Na and heat fluxes at McMurdo peak near 84 km with values of
129 about $-5.5 \times 10^4 cm^{-2}s^{-1}$ and $-3.0 Km/s$, respectively, compared to ~ 88 km at mid-latitudes
130 with values about one half to one third as large for the Na flux. We hypothesize that these
131 differences are caused by strong downwelling over the polar cap at this time of year and strong
132 atmospheric mixing by both dissipating and non-dissipating gravity waves, including the long-
133 period persistent gravity waves discovered at McMurdo (Chen et al., 2013, 2016).

134 **2. McMurdo Lidar Data Acquisition and Processing**

135 The McMurdo lidar campaign was conducted by the University of Colorado Boulder
136 through a collaboration between the United States Antarctic Program (USAP) and Antarctica
137 New Zealand (AntNZ) (Chu, Huang, et al., 2011; Chu, Yu, et al., 2011). The STAR (Student
138 Training and Atmospheric Research) Na Doppler lidar was installed into the AntNZ laboratory at
139 Arrival Heights Observatory ($77.84^\circ S$, $166.67^\circ E$) in Jan 2018 (Chu et al., 2020), where it has
140 since been operated alongside an Fe Boltzmann temperature lidar (not used in this study) that
141 was installed in 2011. McMurdo is located at the edge of polar cap and auroral oval (Fong et al.,
142 2014, 2015), and it is also a hotspot for gravity waves (Chen et al., 2013, 2016; Chen & Chu,
143 2017; Zhao et al., 2017; Chu et al., 2018) and planetary waves (Lu et al., 2013, 2017a). Long
144 dark nights in winter months enable the Na lidar to make high-resolution measurements of Na,

145 temperature, and vertical winds covering the complete temporal spectrum of gravity waves from
146 the buoyancy period (~ 5 min) to the inertial period (~ 12.3 h).

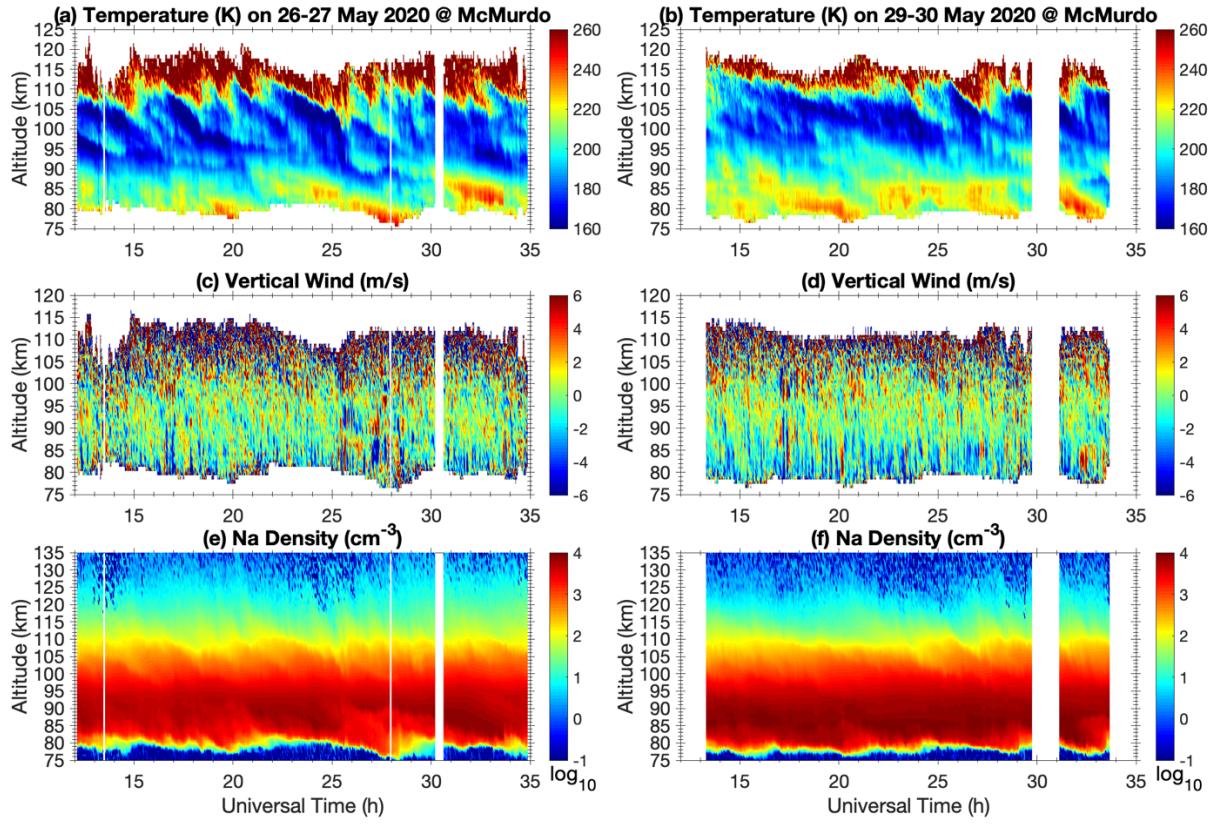
147 The STAR Na lidar employs the 3-frequency ratio technique to infer simultaneously the
148 temperature (T), vertical wind (w), and atomic Na number density (ρ_{Na}) in the MLT region (e.g.,
149 Chu & Papen, 2005). The laser transmitter operates at the Na D_{2a} wavelength of 589.15826 nm
150 and at a pulse repetition rate of 50 pps with a single pulse energy of ~ 10 –20 mJ. The local
151 oscillator laser is frequency-locked to the D_{2a} peak frequency by employing saturation-
152 absorption spectroscopy, and then the output beam is frequency-shifted by ± 750 MHz using dual
153 acousto-optic modulators to achieve 3-frequency operation (e.g., She & Yu, 1994). With an 81-
154 cm diameter Newtonian telescope, the STAR lidar power-aperture product (PA) is between 0.25
155 and 0.5 Wm². The photo detector is a Hamamatsu H7421–40 photomultiplier tube (PMT,
156 modified version) with a quantum efficiency (QE) of 40%. The high-efficiency receiver
157 architecture (Smith & Chu, 2015), coupled with the high-QE PMT, produces large signal counts
158 enabling high-resolution measurements even at the edges of the Na layer. For the data employed
159 in this study, the Na densities, and hence the signal levels, varied over a dynamic range of more
160 than 3 orders of magnitude. The PMT response curve was carefully measured and calibrated over
161 this wide dynamic range to eliminate signal distortion caused by PMT nonlinearities, which, if
162 not corrected, can affect heat flux measurements, especially at very high signal levels sometimes
163 encountered near the peak of the Na layer (Liu & Guo, 2016). Detailed system specifications can
164 be found in the Supporting Information of Chu et al. (2020).

165 The lidar data acquisition (DAQ) system saves the 3-frequency raw photon counts at
166 fundamental resolutions of 4.5 s (1.5 s per frequency) in time (t) and 24 m in altitude (z). In post
167 processing, the odd and even photon count samples in time are integrated separately to achieve
168 the desired temporal and vertical resolutions, which for this study are $\Delta t = 2.5$ min and $\Delta z =$
169 0.96 km. This yields two statistically independent photon count profiles for each of the 3 laser
170 frequencies that are interleaved in time and offset by the 4.5 s fundamental temporal resolution.
171 Note, by independent, we mean that the photon noise contaminating each of the profiles is
172 uncorrelated with the noise contaminating any other profile. However, because of the small 4.5 s
173 offset, the gravity wave fluctuations that perturb the two interleaved photon count profiles are
174 virtually perfectly correlated. This is equivalent to probing the same region of the atmosphere

175 with two different lidars. The interleaved profiles are added when deriving the basic atmospheric
176 parameters of T , w , and ρ_{Na} along with their uncertainties (ΔT , Δw , and $\Delta \rho_{Na}$). However, to
177 eliminate photon noise biases when computing variances and fluxes, two statistically
178 independent profiles of T , w , and ρ_{Na} are derived from the interleaved photon counts, which are
179 then used to compute independent profiles of w' , T' , and ρ'_{Na} , where the prime denotes the
180 fluctuation quantity. These independent fluctuation profiles are used to compute the variances
181 and fluxes as described by Gardner and Chu (2020). This interleaved approach eliminates the
182 photon noise biases and produces accurate estimates of variances and fluxes, provided the
183 number of data samples is sufficiently large, which is the case for McMurdo Na Doppler lidar
184 dataset. Bias elimination is especially important in enabling the flux and fluctuation variance
185 measurements to be extended into the thermosphere above 100 km and below 85 km where
186 measurement uncertainties increase substantially because of the low signal levels caused by
187 decreasing Na densities.

188 **3. Fundamental Atmospheric Observations**

189 Observations of MLT temperatures, vertical winds, and Na densities on 26–27 May 2020
190 and 29–30 May 2020 at McMurdo are illustrated in Figure 1. The mean temperature (\bar{T}), lapse
191 rate ($-\partial \bar{T} / \partial z$), and Na density ($\bar{\rho}_{Na}$) profiles and their errors are plotted in Figure 2. A striking
192 feature is the rich spectrum of gravity waves. Temperature perturbations are dominated by
193 persistent, low-frequency gravity waves with periods of 3–10 h (Chen et al., 2016; Chen & Chu,
194 2017), while vertical wind perturbations are dominated by high-frequency gravity waves with
195 periods less than ~ 1 h. These high-frequency waves are clearly visible in the temperature
196 contours but with much smaller amplitudes than the persistent waves. Similarly, the low-
197 frequency waves are visible in the vertical wind contours but with smaller amplitudes. This is
198 consistent with the gravity wave polarization relations $|w'| \simeq \frac{\omega g}{N^2} \frac{|T'|}{\bar{T}}$, where ω is the intrinsic
199 frequency, $g = 9.5 \text{ m/s}^2$ is the gravitational acceleration, and $N \simeq 2\pi/5 \text{ min}$ is the buoyancy
200 frequency, so that the vertical wind perturbations increase with increasing intrinsic frequency.
201 Note, the measurements illustrated in Figure 1 include the Doppler effects associated with the
202 background wind field. Hence, the parameter fluctuation spectra represent the observed, not the
203 intrinsic, frequencies, which under certain circumstances can be substantially different and where
204 downward phase progression does not necessarily indicate upward energy propagation.

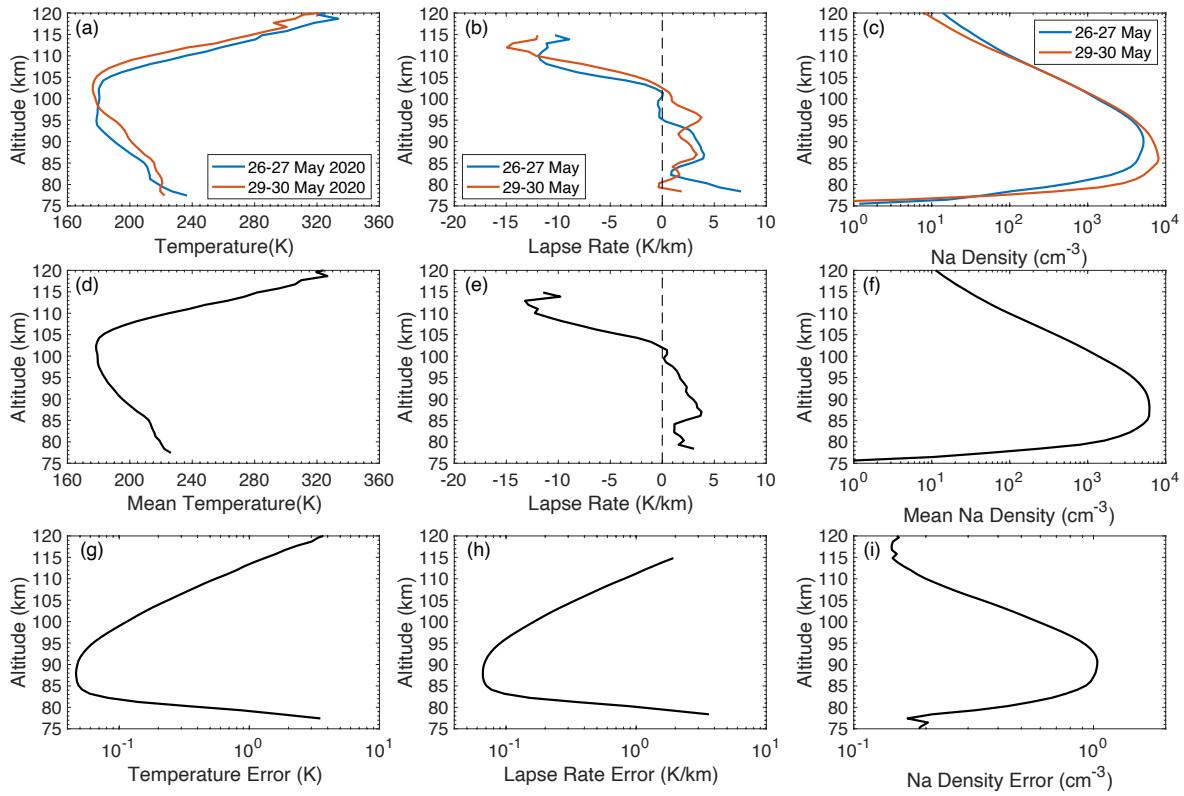


205

206 *Figure 1. Contour plots of (top) temperature, (middle) vertical wind, and (bottom) Na density*
 207 *observed in the MLT at McMurdo, Antarctica during 26–27 and 29–30 May 2020 with the*
 208 *University of Colorado Na Doppler lidar. The data resolutions are $\Delta t = 2.5$ min and $\Delta z =$*
 209 *960 m. The Na density is plotted in log-10 scale. The upward wind is positive.*

210 Another interesting feature observed in Figure 2c is the low peak altitudes of Na layers.
 211 Both lidar runs show the Na layer peak below 90 km, and the peak on 29–30 May 2020 is close
 212 to 85 km. The Na layers measured at midlatitudes have peaks usually above 90 km, even during
 213 winter (e.g., Gardner & Liu, 2010; Guo & Liu, 2021). Furthermore, the Na layers at McMurdo
 214 extend below 80 km, giving sufficient signal for deriving temperature and vertical wind below
 215 80 km. This situation is very different from the midlatitude observations where Na signals
 216 typically fall quickly below 85 km. The layer bottom side extension at McMurdo is clearly
 217 illustrated in Figures 2c and 2f. Even at 78 km, the mean Na density is still above 100 cm^{-3} ,
 218 enabling the measurements of temperature and its lapse rate. The Na layer peak altitude on 26–
 219 27 May 2020 is higher than on 29–30 May 2020, but both runs exhibit small temperature
 220 inversion layers with the peak inversion around 84–85 km (Figure 2a), which, as discussed later,

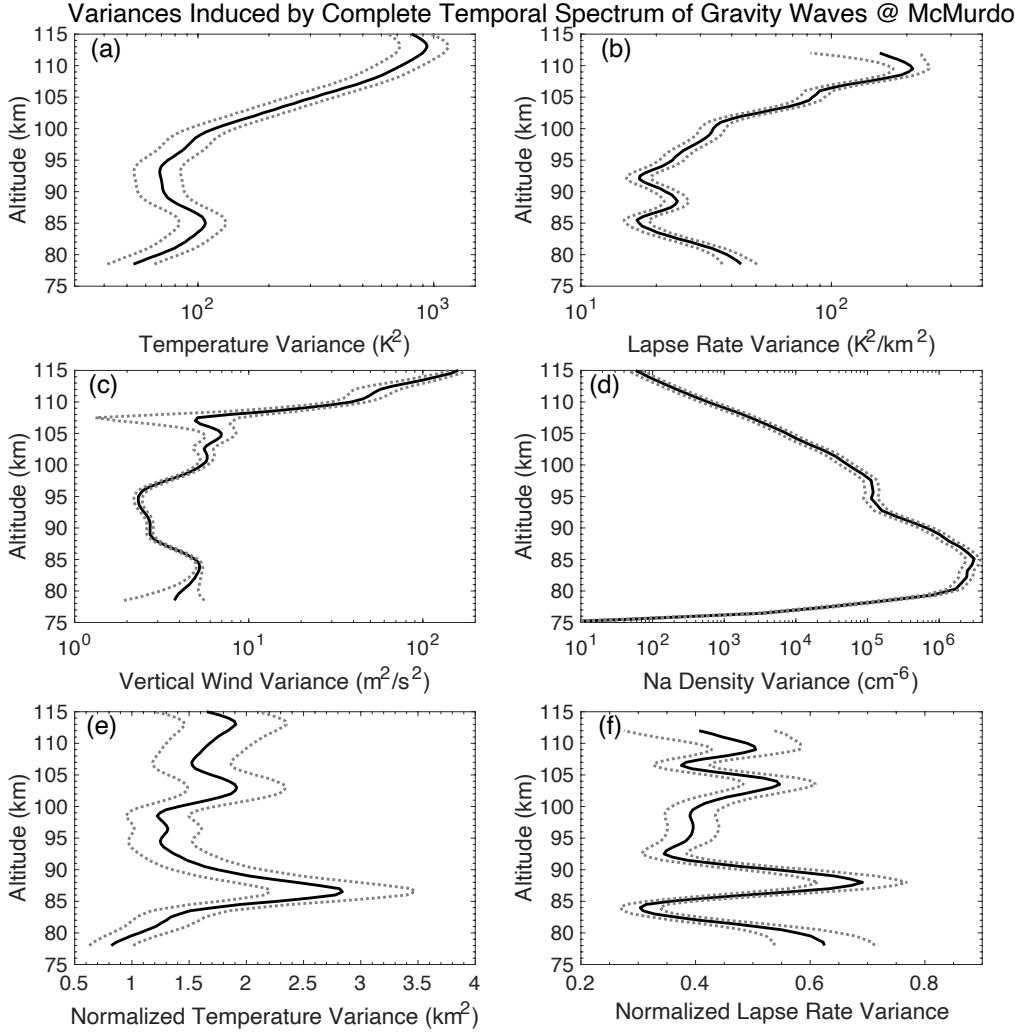
221 may be associated with wave dissipation and heat transport. For the overall mean temperature
 222 profile in Figure 2d, the mesopause is located at 102.4 km and there is a small inversion peak at
 223 85 km, which causes a sharp increase in the environmental lapse rate above 85 km. The lapse
 224 rate ($-\partial\bar{T}/\partial z$) of the overall mean temperature is positive below the mesopause but becomes
 225 negative and grows quickly above the mesopause. The small temperature inversion layer leads to
 226 the largest lapse rate of about 4 K/km at 86.5 km. It is worth noting that simultaneous
 227 measurements by the Fe Boltzmann lidar show the same mesopause features and temperature
 228 inversion layers around 85 km, while the observed Fe layers (not shown) also exhibit low peak
 229 altitudes and downward extension of the layer bottom sides like the Na layers.



230

231 *Figure 2. Profiles of (a) mean temperature, (b) lapse rate, and (c) Na density observed in the*
 232 *MLT at McMurdo, Antarctica during 26–27 and 29–30 May 2020 with the University of*
 233 *Colorado Na Doppler lidar. Profiles of the overall mean temperature (\bar{T}), lapse rate ($-\partial\bar{T}/\partial z$),*
 234 *and Na density ($\bar{\rho}_{\text{Na}}$) profiles and their rms uncertainties are plotted in (d)–(i). The lapse rate*
 235 *profiles in (b) and (e) were smoothed with a Hamming window with a full width of 2.5 km.*

Figures 3a–3d illustrate the variances of temperature, environmental lapse rate, vertical wind, and Na number density perturbations in the MLT that were induced by the complete temporal spectrum of gravity waves. As discussed in Section 2, to eliminate photon noise biases, which can be especially large at the extreme altitudes where the signal levels are small, these variance profiles were derived using the interleaved datasets according to the processing procedure described by Gardner and Chu (2020). The temperature, vertical wind, and Na density fluctuations were computed by subtracting the temporal means for each of the two observation periods. The variance profiles have been smoothed using a Hamming window with a full width of 5 km to reduce the uncertainties, especially the contributions from photon noise (see Supporting Information for plots of the unsmoothed profiles). The smoothed variance profiles include the unattenuated contributions from waves with vertical wavelengths as small as $2\Delta z = 1.92 \text{ km}$, but the resolution of variance profiles has been reduced to about 3.42 km (rectangular window equivalent) by applying the Hamming window smoothing function. The root-mean-square (rms) uncertainties (error bars) were computed according to Appendix B and plotted as gray-dotted curves in Figure 3. We also computed and plotted the normalized temperature and lapse rate variances in Figures 3e and 3f, where the normalization factor is $(\Gamma_{ad} + \partial\bar{T}/\partial z)^2$, $\Gamma_{ad} = g/C_p$ is the dry adiabatic lapse rate, and $C_p = 1003 \text{ m}^2 \text{K}^{-1} \text{s}^{-2}$ is the specific heat at constant pressure. The normalized temperature variance is approximately equal to the mean-square value of the displacements imparted to the atmosphere by the spectrum of waves. It is correlated with the strength of the vertical wind fluctuations and is therefore a measure of the degree of vertical mixing induced by the waves. The normalized lapse rate variance is approximately equal to the mean of the inverse Richardson number (Ri) and is a measure of the instability of the atmosphere through which the waves are propagating (see Appendix A, Equation (A9)). These normalized, fluctuation variance profiles suggest that between 86 and 92 km is a region of high instability and vigorous atmospheric mixing. Notice that the temperature contours in Figure 1 are disorganized in this region but exhibit distinct wave signatures with downward phase progression above and below. The normalized variances will be used later to calculate the gravity wave potential energy per unit mass (E_{pm}) and to estimate the fraction of wave energy propagating downward (α_{down}).



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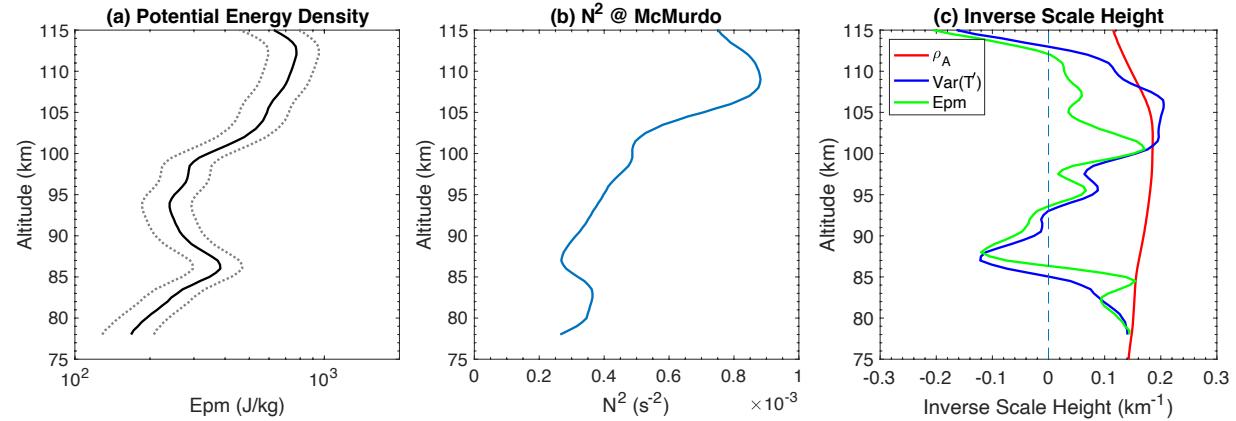
266 *Figure 3. Profiles of the computed fluctuation variances of (a) temperature $\text{Var}(T') = \overline{(T')^2}$, (b)*
 267 *lapse rate $\text{Var}(-\partial T'/\partial z) = \overline{(\partial T'/\partial z)^2}$, (c) vertical wind $\text{Var}(w') = \overline{(w')^2}$, and (d) Na density*
 268 *$\text{Var}(\rho'_{Na}) = \overline{(\rho'_{Na})^2}$ induced by the complete temporal spectrum of gravity waves in the MLT at*
 269 *McMurdo, Antarctica during 26-27 and 29-30 May 2020. Profiles of the (e) normalized*
 270 *temperature variance $\text{Var}(T')/(\Gamma_{ad} + \partial \bar{T}/\partial z)^2$ and (f) normalized lapse rate variance*
 271 *$\text{Var}(-\partial T'/\partial z)/(\Gamma_{ad} + \partial \bar{T}/\partial z)^2$. The profiles were smoothed with a 5 km full width Hamming*
 272 *window. The rms uncertainties (error bars) are plotted as gray-dotted curves.*

273 The temperature variance $\text{Var}(T')$ profile in Figure 3 exhibits a local maximum (peak) of
 274 $\sim 110 \text{ K}^2$ at $\sim 85 \text{ km}$ where the small peak of the temperature inversion is located in Figure 2. A
 275 minimum lapse rate variance $\text{Var}(-\partial T'/\partial z)$ of $\sim 14 \text{ K}^2/\text{km}^2$ and a maximum Na density
 276 variance $\text{Var}(\rho'_{Na})$ of $\sim 3.1 \times 10^6 \text{ cm}^{-6}$ occur at similar altitudes. The vertical-wind variance

277 $Var(w')$ has a local maximum of $5.7 \text{ m}^2/\text{s}^2$ around 84 km. After a decrease above 85 km, the
278 temperature variance starts to increase above 94 km and grows rapidly above 100 km, alongside
279 the growth of the lapse rate variance. The potential energy per unit mass E_{pm} of the gravity wave
280 spectrum is computed from the temperature variance and square of buoyancy frequency (N^2)
281 measured by the lidar

282
$$E_{pm} \simeq \frac{1}{2} \frac{g^2}{N^2 \bar{T}^2} \overline{(T')^2} = \frac{N^2}{2} \frac{Var(T')}{(\Gamma_{ad} + \partial \bar{T} / \partial z)^2}. \quad (1)$$

283 Although we use this expression for E_{pm} , its validity diminishes for the highest wave frequencies
284 near the buoyancy frequency, which our data include. The E_{pm} and N^2 profiles are shown in
285 Figures 4a and 4b, respectively. The inverse scale heights for the atmospheric density (red
286 curve), $Var(T')$ (blue curve) and E_{pm} (green curve) are plotted for comparison in Figure 4c. The
287 atmospheric density profile, used to calculate the scale height, was obtained from the atmosphere
288 model NRLMSISE-00 (Picone et al., 2002). As expected for dissipating gravity waves, the
289 inverse scale heights for $Var(T')$ and E_{pm} are smaller than for ρ_A throughout most of the range
290 between 80 and 115 km. In fact, dissipation is so strong between 86 and 92 km and above 112
291 km that the inverse scale heights are negative, reflecting the reduction of wave amplitudes with
292 increasing altitude in these regions. The high instability and vigorous mixing (as indicated by the
293 normalized variances of lapse rate and temperature in Figure 3) along with the local minima of
294 $Var(T')$ and E_{pm} and the negative scale heights suggest that the strongest wave dissipation and
295 gravity wave breaking occur in this region of ~ 86 –92 km. However, near 100 km, all three
296 inverse scale heights are comparable indicating negligible wave dissipation, while between 101
297 and 108 km the temperature variance increases faster than $1/\rho_A$ which may be an indication that
298 some waves are being amplified (Fong et al., 2014, 2015; Lu et al., 2017a). Although the
299 evidence suggests that dissipation is the primary source of E_{pm} decay between 86 and 92 km, as
300 noted by a reviewer, other potential channels for the decrease (or increase) in E_{pm} are the
301 conversions between wave potential and kinetic energies and between wave potential energy and
302 the mean potential energy. Both conversions are driven by the potential temperature flux and can
303 proceed either way.



304

305 *Figure 4. Profiles of the (a) potential energy per unit mass, (b) square of buoyancy frequency,*
 306 *and (c) inverse scale heights of atmospheric density, temperature variance, and potential energy*
 307 *per unit mass for the MLT above McMurdo in Late May 2020. The E_{pm} and N^2 profiles were*
 308 *smoothed with a 5 km full-width Hamming window and the inverse scale heights were computed*
 309 *from smoothed profiles. The rms uncertainties (error bars) of E_{pm} are plotted as gray-dotted*
 310 *curves in (a).*

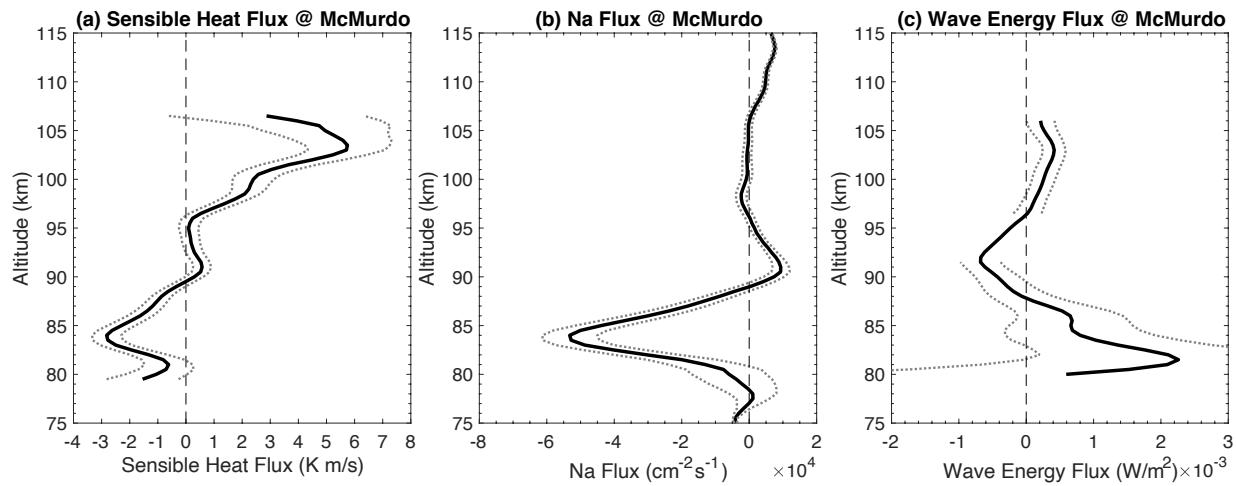
311 The E_{pm} profile in Figure 4a exhibits a striking similarity in shape to the E_{pm} profile
 312 published in Figure 20 of Vadas and Becker (2019). These authors used numerical modeling to
 313 explore secondary and tertiary gravity wave generation over the Southern Andes. Their E_{pm}
 314 profile was derived by averaging the modeled, wave-driven potential energy density over the
 315 region from 279–296°E and 55.1–29.6°S for July 23 (mid-winter). In Vadas and Becker (2019),
 316 E_{pm} increases from the troposphere with increasing altitude, reaching a local maximum at ~85
 317 km (like McMurdo), and then decreases in the height range between ~85 and ~94 km (also like
 318 McMurdo). The authors attribute the decrease to the breaking of primary waves that were
 319 launched in the lower atmosphere, which leads to the generation of secondary waves in the
 320 mesopause region. Above ~94 km, the amplitudes of the secondary waves increase with
 321 increasing altitude and reach another local maximum at ~112 km (like McMurdo). The decrease
 322 of E_{pm} between ~115–125 km occurs where most of the secondary gravity waves dissipate,
 323 leading to the generation of tertiary gravity waves (Vadas & Becker, 2019). Above McMurdo,
 324 the measured E_{pm} profile also exhibits local maxima at ~85 and ~112 km which is quite similar
 325 to the Vadas and Becker (2019) results, although the measured McMurdo E_{pm} at 112 km is
 326 about half the modeled value for the Southern Andes region. Such similarities suggest that

secondary and tertiary gravity waves are also generated in the MLT above McMurdo via the multistep vertical coupling process that was proposed by Vadas and Becker (2018 & 2019). Because the secondary and tertiary waves propagate both upward and downward, this mechanism could potentially lead to substantial fractions of downward-propagating gravity waves throughout the MLT region at McMurdo.

4. Vertical Flux Observations

The vertical fluxes of sensible heat ($\overline{w'T'}$) and Na density ($\overline{w'\rho'_{Na}}$) were computed using the interleaved data at resolutions of $\Delta z = 0.96 \text{ km}$ and $\Delta t = 2.5 \text{ min}$ and then averaged over the two observation periods. This approach eliminates the small biases associated with partially correlated photon noise errors in the derived values of w' , T' and ρ'_{Na} (Gardner & Chu, 2020). The results are plotted in Figure 5 after vertically smoothing using a Hamming window with a full width of 5 km (see Supporting Information for plots of the unsmoothed profiles). Because the resolution of the lidar data processing excluded the smaller-scale turbulence fluctuations, these profiles represent the vertical fluxes induced by gravity waves (not turbulence) with vertical wavelengths greater than $2\Delta z = 1.92 \text{ km}$ and frequencies spanning the full temporal spectrum from f to N , in the region below 100 km, where the buoyancy period is 5 min or longer. Above 100 km, where the buoyancy period is as short as 3.5 min (@110 km), the data exclude the highest frequency waves. However, the temperature, Na, and horizontal wind spectra are dominated by medium- and low-frequency waves, so the missing high-frequency wave energy is small. The data were not high-pass filtered so the fluxes may also include contributions from tides and planetary waves with periods up to $\sim 40 \text{ h}$, although because of their small vertical wind and temperature amplitudes, those contributions should be insignificant. The measurements exclude the smaller flux contributions from eddy and molecular diffusion which were not resolved. The Na flux is generally downward with the largest negative values between 80 and 90 km and a maximum value of about $-5.5 \times 10^4 \text{ cm}^{-2} \text{ s}^{-1}$ at 84 km where the sensible heat flux also exhibits its maximum downward value of about -3.0 Kms^{-1} . This altitude range of 80–90 km is a region of enhanced wave dissipation, which contains the local maxima in the temperature variance, normalized temperature variance, normalized lapse rate variance, and E_{pm} (Figures 3a, 3e, 3f, and 4a).

356

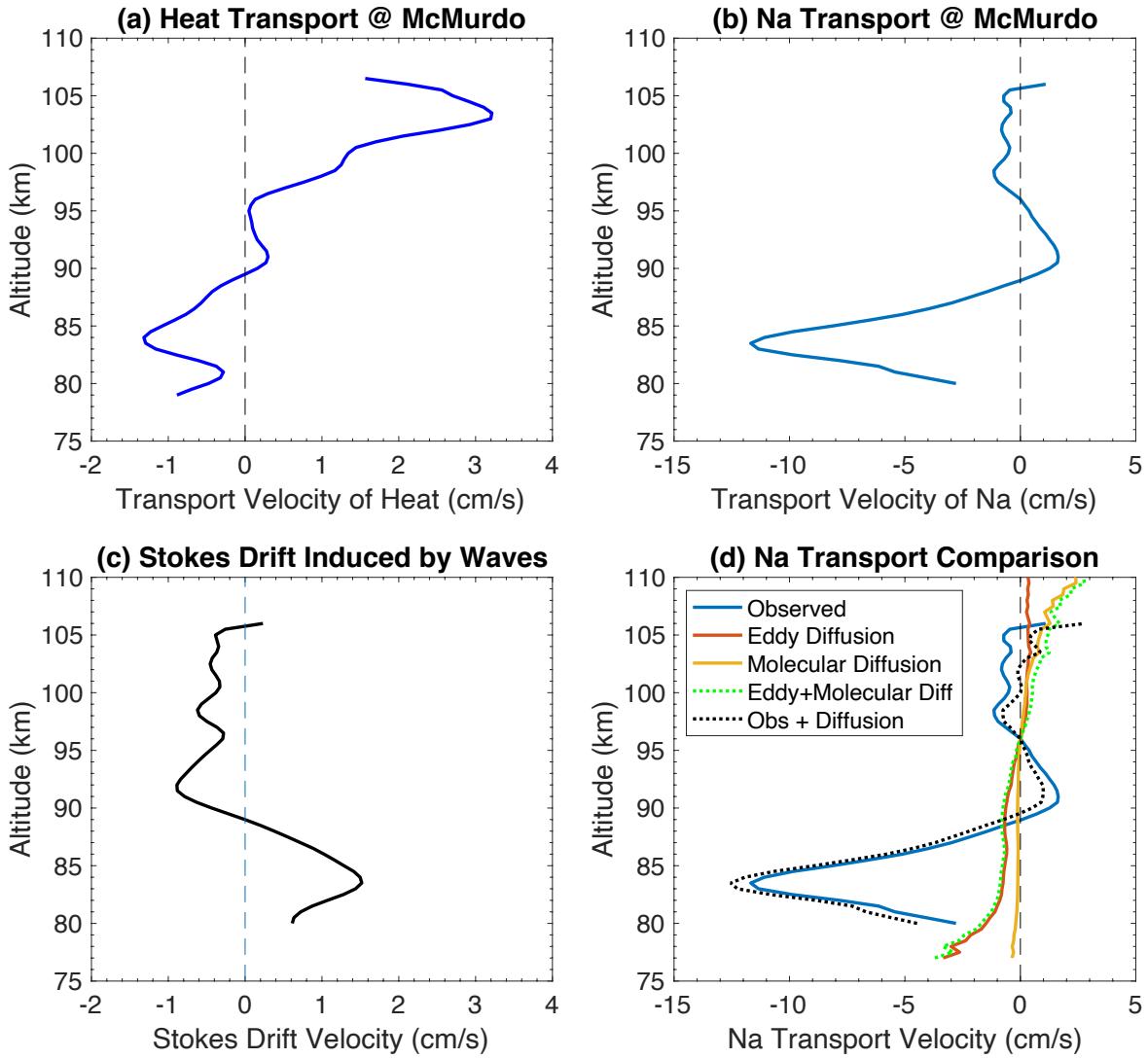


357

358 *Figure 5. Profiles of the vertical fluxes of (a) sensible heat ($\overline{w'T'}$), (b) Na ($\overline{w'\rho'_{Na}}$), and (c)*
 359 *gravity wave energy ($\overline{w'p'}$) observed in the MLT at McMurdo in late May 2020. The rms*
 360 *uncertainties (error bars) of fluxes are plotted as gray-dotted curves. The energy flux profile was*
 361 *derived from the measured heat and Na flux profiles and by using the mean pressure profile from*
 362 *the atmospheric model NRLMSISE-00 (Picone et al., 2002).*

363

364 The wave-induced, vertical transport velocities of sensible heat $\overline{w'T'}/\bar{T}$ and Na
 365 $\overline{w'\rho'_{Na}}/\bar{\rho}_{Na}$ are plotted in Figures 6a and 6b. The heat transport velocity profile exhibits a
 366 downward peak of -1.3 cm/s at 84 km and an upward peak of $+3.2 \text{ cm/s}$ at 103 km . In
 367 comparison, the downward Na transport velocity reaches -11.7 cm/s at $\sim 84 \text{ km}$, which is more
 368 than double of the peak values observed at midlatitudes. The Na transport is slow and upward
 369 (positive) from 89 to 96 km and the small values are less than 2 cm/s . From 97 to 106 km , the Na
 370 transport is slightly downward with small values about -1 cm/s . Note that the transport
 371 velocities shown in Figure 6 are the velocities relative to the background atmosphere, not relative
 372 to the ground. This is because the background vertical wind has been subtracted in the derivation
 373 of w' and the fluxes.



374

375 *Figure 6. (a) Transport velocity of heat, and (b) Na, and (c) the Stokes drift velocity induced by*
 376 *the complete temporal spectrum of gravity waves at McMurdo in late May 2020. (d) Comparison*
 377 *of the observed Na transport velocity induced by non-breaking gravity waves with those induced*
 378 *by molecular and eddy diffusion.*

379 Heat and/or Na flux observations have been reported from six sites in both the northern
 380 and southern hemispheres and the key results are summarized in Table 1. Compared to other
 381 observations made at mid-latitudes in both hemispheres, the heat and Na fluxes at McMurdo
 382 reach their maximum downward values at a considerably lower altitude and for the Na flux, the
 383 magnitude is larger. The seasonal variations of sensible heat flux at the Starfire Optical Range,
 384 NM (SOR, 35°N) exhibit strong semi-annual variations with maximum downward values of -2

385 to -3 K m/s at about 88 km altitude from early Nov to early Feb and minimum values of about
386 -0.5 K m/s at the equinoxes (Gardner & Liu, 2007). The Na flux at SOR also exhibits strong
387 semi-annual variations with maximum values ranging from $-1.75 \times 10^4 \text{ cm}^{-2} \text{s}^{-1}$ to
388 $-2.75 \times 10^4 \text{ cm}^{-2} \text{s}^{-1}$ at 88 km, from early Nov to early Feb and minimum values of about
389 $-0.25 \times 10^4 \text{ cm}^{-2} \text{s}^{-1}$ at the equinoxes (Gardner & Liu, 2010). The late May McMurdo
390 observations reported here correspond to late Nov measurements at SOR. The heat flux values
391 for late fall are comparable at the two sites, but the peak altitude is about 4 km lower at
392 McMurdo, which may simply reflect the stronger wintertime downwelling induced by the
393 (residual) meridional circulation system at this high polar latitude. The peak value of the
394 downward Na flux at McMurdo is more than twice the value observed at SOR, even though the
395 Na density at 84 km at McMurdo in late May ($\sim 5000 \text{ cm}^{-3}$) is somewhat smaller than the Na
396 density at 88 km at SOR in late Nov ($\sim 6500 \text{ cm}^{-3}$). As will be discussed in Section 6, the larger
397 Na flux at McMurdo appears to be associated with more intense wave activity as reflected in
398 variance of the temperature fluctuations ($\sim 105 \text{ K}^2$ @ 84 km for McMurdo versus $\sim 60 \text{ K}^2$ @ 88
399 km for SOR). This is not surprising since the McMurdo Na flux measurements include the
400 contributions from the complete temporal spectrum of gravity waves, while the SOR Na flux
401 excludes the effects of the longer period waves, viz. waves with periods exceeding the mean
402 observation period of $\sim 7.6 \text{ h}$.

403 Recently, Guo and Liu (2021) reported seasonal variations of the vertical gravity wave
404 heat flux at Cerro Pachón, Chile (CP, 30°S). The measured sensible heat flux reveals strong
405 annual and weak semi-annual oscillations, with the maximum downward fluxes observed in mid-
406 winter during Jun and Jul. The heat flux profile exhibits a broad maximum in late June extending
407 from about 88 to 94 km with values averaging about -2.5 Kms^{-1} , similar to the peak value
408 observed in late May at McMurdo. In contrast, observations at Hefei, China (31.5°N) in the fall,
409 revealed a maximum downward heat flux at 88 km of only -0.3 Kms^{-1} and maximum
410 downward Na flux at 89 km of only $-0.3 \times 10^4 \text{ cm}^{-2} \text{s}^{-1}$ (Tao Li, private communication,
411 University of Science and Technology of China). These small flux values may reflect significant
412 differences in wave activity at Hefei compared to SOR and CP, and as we will show later, may
413 also be related to temporal resolution with which the data were acquired. Heat and Na flux
414 measurements were also made at Maui, HI (20.7°N). The annual mean heat flux profile exhibited
415 two downward maxima of -1.25 Kms^{-1} at 87 km and -1.4 Kms^{-1} at 95 km. The annual mean

416 Na flux exhibited a downward maximum of $-0.8 \times 10^4 \text{ cm}^{-2} \text{s}^{-1}$ at 87 km. Finally, Na flux
 417 observations at Table Mt., CO (40°N, Huang et al., 2015) in Aug and Sep (corresponds to Feb
 418 and Mar at McMurdo) had a peak value at 86 km of $-1.5 \times 10^4 \text{ cm}^{-2} \text{s}^{-1}$. In summary, the
 419 McMurdo heat and Na fluxes reach their maximum downward values ~4 km lower in altitude
 420 than the mid-latitude observations. The peak value of heat flux at McMurdo is comparable to the
 421 largest values observed at SOR and Cerro Pachón, while the peak Na flux value is the largest by
 422 about a factor of 2.

423 **Table 1 Summary of Sensible Heat and Na Flux Observations in the Mesopause Region**

Site	Table Mountain, Colorado	SOR, New Mexico	Hefei, China	Maui, Hawaii	Cerro Pachón, Chile	McMurdo, Antarctica
Reference	Huang et al. (2015)	Gardner & Liu (2007 & 2010)	Tao Li (Private Comm.)	Liu & Gardner (2005)	Guo & Liu (2021)	This Paper
Latitude	40.1°N	35.0°N	32°N	20.7°N	30.25°S	77.84°S
Longitude	105°W	106.5°W	117°E	156.3°W	70.74°W	166.7°E
Inertial Period (h)	18.6	20.9	22.6	33.9	24.0	12.3
Observation Length (h)	~5	~7.6	~10	~6.6	~5	~20
Observation Period	Aug/Sep	Late Nov	Fall Mean	Annual Mean	June	Late May
Time Resolution Δt (min)	10	1.5	10	1.5	1	2.5
Alt. Resolution Δz (km)	0.96	0.5	~3	0.96	2	0.96
Heat Flux Peak (K m/s)	N/A	-2.5	-0.3	-1.4	-2.8	-3.0
Heat Flux Peak Altitude (km)	N/A	88	88	87–95	88–94	84
Na Flux Peak ($10^4 \text{ cm}^{-2} \text{s}^{-1}$)	-1.5	-2.25	-0.3	-0.8	N/A	-5.5
Na Flux Peak Altitude (km)	86	88	89–95	88	N/A	84

424 Between 95 and 106 km the heat flux at McMurdo is positive, which suggests that wave
 425 dissipation is relatively weak at these higher altitudes near the mesopause where the atmosphere
 426 becomes more stable as the environmental lapse rate decreases to zero at the mesopause (102.4

427 km) and then becomes negative in the lower thermosphere. By comparison, the heat flux is also
 428 positive in the thermosphere at SOR above 95 km from April through October when the
 429 mesopause is located near 86 km (Chu et al., 2005), reaching values of +1 Km/s near 100 km
 430 (Gardner & Liu, 2007). Because the McMurdo heat flux measurements are the first to be
 431 reported from above 100 km, there are no other observations in this region and so we compare
 432 the measurements with theory.

433 Wave dissipation can be quantified by calculating the potential temperature flux,

$$434 \quad \frac{\overline{w'\theta'}}{\theta} = \frac{\overline{w'T'}}{\bar{T}} - \kappa \frac{\overline{w'p'}}{\bar{p}} = -\frac{1}{\theta} \frac{\partial \bar{\theta}}{\partial z} K_H \quad (2)$$

435 where potential temperature $\theta = T \left(\frac{p_0}{p} \right)^\kappa$, $\kappa = R/C_p$, $R = 287 \text{ m}^2 \text{K}^{-1} \text{s}^{-2}$ is the gas constant for
 436 dry air, $C_p = 1,003 \text{ m}^2 \text{K}^{-1} \text{s}^{-2}$ is the specific heat at constant pressure, p is the atmospheric
 437 pressure, and $\overline{w'p'}$ is the gravity wave energy flux. The right-hand-side of (2) follows by
 438 invoking Fick's First Law of Diffusion of θ , where in this case K_H is the effective thermal
 439 diffusivity induced by non-breaking wave motions. By solving (2) for $\overline{w'T'}$ and noting that
 440 $\frac{1}{\theta} \frac{\partial \bar{\theta}}{\partial z} = \frac{N^2}{g}$, we obtain

$$441 \quad \overline{w'T'} = (\Gamma_{ad} + \partial \bar{T} / \partial z)(K_E - K_H), \quad (3)$$

442 where for convenience we define K_E as the effective diffusivity associated with the gravity wave
 443 energy flux $\overline{w'p'}$

$$444 \quad K_E = \kappa \frac{g}{N^2} \frac{\overline{w'p'}}{\bar{p}}. \quad (4)$$

445 Potential temperature is a conserved quantity for an air parcel in adiabatic motion, that is,
 446 for motion in which there are no heat sources or sinks. Although we believe that this condition
 447 may be violated in the lower thermosphere above McMurdo, for the moment let us assume that
 448 adiabatic motion applies. We also assume that in the absence of wave dissipation, the wave-
 449 induced potential temperature flux and K_H are zero. In this case, according to (3), the sensible
 450 heat flux is proportional to K_E and the energy flux ($\overline{w'p'} = \frac{N^2 \bar{p}}{g \kappa} K_E$), which is positive for regions
 451 dominated by upward-propagating gravity waves. At 103 km, where the positive sensible heat

452 flux at McMurdo reaches $5.5 \pm 1.5 \text{ Km/s}$, if $K_H \simeq 0$ then $K_E = 580 \pm 160 \text{ m}^2/\text{s}$ and $\overline{w'p'} =$
453 $2.2 \pm 0.6 \text{ mW/m}^2$. In the following section we show that these large values for K_E and $\overline{w'p'}$ are
454 possible according to the gravity wave polarizations relations (Vadas, 2013), especially when the
455 wave spectrum is dominated by upward-propagating waves with the amplitudes and phase
456 speeds that are commonly observed in the lower thermosphere. However, we believe that there
457 may be other factors involved, which could potentially lead to negative values for K_H and large
458 positive values for the sensible heat flux. These factors include the amplification of inertial
459 period waves, which has been observed for tides and planetary waves in this region above
460 McMurdo (Fong et al., 2014, 2015; Lu et al., 2017a). Additionally, heat sources associated with
461 the aurora in the lower thermosphere, may also affect the phase shift between w' and T' , which
462 could lead to large positive heat flux values. Coupled with the severe dissipation of primary
463 gravity waves around 85–95 km, the observed profile of sensible heat flux transitioning from
464 downward below 90 km to upward from 97 to 106 km can be explained in terms of the
465 generation of secondary gravity waves and the gravity wave polarization relations. The
466 comparison of the measured heat flux with theory is detailed in Section 5 and the impact of
467 secondary waves is further examined in Section 6.

468 **5. Comparison of the Measured Heat and Estimated Energy Fluxes with Theory**

469 The large positive sensible heat flux from 97 to 106.5 km differs from the conventional
470 understanding of wave-driven atmospheric motions, in which the sensible heat flux induced by
471 gravity waves is expected to be either zero for conservative waves or negative for dissipating
472 waves regardless of the wave propagation direction (Walterscheid, 1981). Although we focus
473 here on the late May 2020 observations, we have observed positive sensible heat fluxes in the
474 lower thermosphere on numerous other winter days, however the magnitudes vary. Positive heat
475 fluxes appears to be a common feature of the lower thermosphere in winter above McMurdo. As
476 shown in Appendix C, the heat and energy fluxes can be directly calculated from the gravity
477 wave polarization relations. For our analysis we employ the compressible, f-plane, non-
478 dissipative polarization relations for w' , T' and p' given by (B11) and (B7) in Vadas (2013).

479 **5.1. Expected Heat and Energy Fluxes from Polarization Relations**

480 For gravity wave oscillations of the form $\exp[i(\omega_r t - kx - ly - mz - \phi)]$, the heat and
 481 energy fluxes, for an individual wave with ground-based frequency ω_r , intrinsic frequency ω ,
 482 and zonal, meridional and vertical wavenumbers of k , l , and m , are given by (see Appendix C)

$$483 \quad \overline{w'(t)T'(t)} = \frac{1}{2} A_w A_T \cos(\phi_w - \phi_T) = -\frac{(\gamma-1)}{2\gamma H} \frac{g}{N^2} \frac{A_T^2}{\bar{T}} \frac{\frac{\omega}{m} \left(1 - \frac{\omega^2}{N^2}\right)}{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2}\right)^2\right]} \quad (5)$$

484 and

$$485 \quad \overline{w'(t)p'(t)} = \frac{1}{2} A_w A_p \cos(\phi_w - \phi_p) = -\frac{\bar{\rho} g^2}{2N^2} \frac{A_T^2}{\bar{T}^2} \frac{\frac{\omega}{m} \left(1 - \frac{\omega^2}{N^2}\right)}{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2}\right)^2\right]}, \quad (6)$$

486 where A_w , A_T , and A_p are the wave amplitudes in w' , T' , and p' , and ϕ_w , ϕ_T , and ϕ_p are the
 487 phases for the maximum fluctuations. $\gamma = C_p/C_v \approx 1.4$ for $z \sim 100 \text{ km}$. The phase differences
 488 are

$$489 \quad \phi_w - \phi_T = \frac{\pi}{2} + \tan^{-1} \left[\frac{1}{mH} \left(\frac{1}{2} - \frac{1}{\gamma} \right) \right] + \tan^{-1} \left[\frac{1}{mH} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2} \right) \right] \quad (7)$$

490 and

$$491 \quad \phi_w - \phi_p = \pi + \tan^{-1} \left[\frac{\gamma-2}{2\gamma mH} \right]. \quad (8)$$

492 Note that for these equations, m is negative (positive) for upward (downward) propagating
 493 waves. These are exact equations which follow from the polarizations relations (Vadas, 2013).
 494 Because w' and T' are nearly 90° out of phase, the sensible heat flux is especially sensitive to the
 495 phase difference between these two parameters. In contrast, because w' and p' are nearly 180°
 496 out of phase, the energy flux is insensitive to the phase difference.

497 To facilitate the discussion below, we rewrite the polarization relation (C-4) here:

$$498 \quad w' = \frac{-ig\omega}{N^2} \frac{\left[1 - \frac{i}{mH} \left(\frac{1}{2} - \frac{1}{\gamma}\right)\right]}{\left[1 + \frac{i}{mH} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2}\right)\right]} \frac{T'}{\bar{T}}. \quad (9)$$

499 Equation (7) is derived directly from this full polarization relation and shows that the phase
 500 difference between w' and T' differs from 90° . That is, $\phi_w - \phi_T < 90^\circ$ for an upward-
 501 propagating, non-dissipative gravity wave with $\omega < N$, and $\phi_w - \phi_T > 90^\circ$ for a downward-
 502 propagating wave with $\omega < N$. Consequently, the sensible heat flux is expected to be positive
 503 and negative for upward and downward propagating waves, respectively.

504 Many researchers employ the Boussinesq approximation ($1 \ll 2mH$) directly to the
 505 polarization relation (9) in their analyses: $w' \simeq \frac{-ig\omega}{N^2} \frac{T'}{\bar{T}}$. In this case the phase difference between
 506 w' and T' is exactly 90° (also see (B-18) in Vadas, 2013), i.e., the last two terms in (7) are
 507 neglected, and so the sensible heat flux $\overline{w'T'}$ is assumed to be zero for non-dissipating waves
 508 regardless of their propagation direction. However, applying the Boussinesq assumption directly
 509 to the polarization relations without distinguishing between the magnitude and phase of the wave
 510 fluctuations, is invalid in the MLT as shown by the right-hand-side of (5) and by (9). Instead,
 511 applying the Boussinesq approximation to the exact expression for the heat flux (but not to the
 512 polarization relations) is valid and we obtain

$$513 \quad \overline{w'(t)T'(t)} \simeq -\frac{1}{2} \frac{g^2 A_T^2}{c_p N^2 \bar{T}^2} \frac{\omega}{m} \left(1 - \frac{\omega^2}{N^2}\right) \simeq -\frac{A_T^2 \omega}{2\bar{T} m}, \quad (10)$$

514 where we note that $\frac{(\gamma-1)}{\gamma} = \frac{R}{c_p}$ and $H = R\bar{T}/g$. For upward propagating, non-dissipating waves
 515 where m is negative, the actual heat flux is positive, not zero, even under the Boussinesq
 516 approximation.

517 Upward-propagating gravity waves with fast vertical phase speeds ($-\omega/m$) and relatively
 518 large temperature amplitudes (A_T) or with slow phase speeds but large temperature amplitudes,
 519 can induce large, positive, sensible heat fluxes. In fact, the sensible heat flux can be quite large
 520 and positive in the lower mesosphere at McMurdo where dissipation is weak and mesoscale
 521 (~ 15 – 30 km) vertical wavelength waves are common (e.g., Chu, Yu, et al., 2011; Chen et al.,
 522 2016; Chen & Chu, 2017). For example, for a vertical wavelength of 20 km and an intrinsic
 523 period of 16.7 min, the intrinsic vertical phase speed (ω/m) is 20 m/s. The mean temperature
 524 was about 175 K at 103 km at McMurdo during our observations, so if the temperature
 525 amplitude of the upward-propagating wave is 5 K, then the wave would induce a positive heat
 526 flux of about $+1.4 \text{ Kms}^{-1}$. According to (7) this corresponds to a phase shift of about -8.6°
 527 from 90° . For persistent gravity waves at McMurdo (Chen et al., 2016), the typical vertical
 528 wavelength and period are 20 km and 5 h, respectively, so the corresponding vertical phase
 529 speed is ~ 1.1 m/s. These lower frequency waves usually have very large amplitudes ~ 20 K at
 530 105 km, so they can contribute positive heat fluxes $\sim + 1.2 \text{ Kms}^{-1}$, which is comparable to the
 531 contribution from the high-frequency waves. If there are on average 3–5 upward-propagating
 532 waves present simultaneously in the lower thermosphere at McMurdo with these average

533 characteristics, then the total heat flux would be $+4$ to $+6 \text{ Kms}^{-1}$, similar to the values
 534 observed. This exercise demonstrates that the predicted phase shift between w' and T' of $\sim 8 -$
 535 9° less than 90° can lead to large, positive sensible heat fluxes induced by upward-propagating,
 536 non-dissipating gravity waves with vertical wavelengths ~ 20 km.

537 The phase difference between w' and T' predicted above from the polarization relations
 538 given in Vadas (2013) are supported by lidar observations of vertical winds and temperatures
 539 over Boulder, Colorado (Lu et al., 2017b). Lu et al. (2017b) measured the phase differences
 540 between w' and T' for 184 mesoscale waves observed between 85 and 100 km at Table Mt., CO.
 541 They found that the mean phase difference $\phi_w - \phi_T = 84.2^\circ$ was 2.6° larger than the phase
 542 difference 81.6° predicted by equation (7), which they showed was likely caused by dissipation
 543 associated with damping by eddy and molecular viscosity (Lu et al., 2017b). To compute the
 544 potential temperature θ flux from the polarization relations, we add additional phase shifts
 545 $\Delta\phi_{w'T'}$ and $\Delta\phi_{w'p'}$ to the phase differences between w' and T' and between w' and p' to
 546 account for dissipation and other effects. As shown in Appendix C, we have

$$547 \quad \overline{w'\theta'} = \bar{\theta} \left(\frac{\overline{w'T'}}{\bar{T}} - \frac{R}{c_p} \frac{\overline{w'p'}}{\bar{p}} \right) \simeq -\frac{g\omega\bar{\theta}}{2N^2} \frac{A_T^2}{\bar{T}^2} \sin(\Delta\phi_{w'T'}). \quad (11)$$

548 The small phase shifts between w' and p' caused by dissipation and other effects are negligible
 549 because these fluctuations are nearly 180° out of phase. In contrast, the small phase shifts
 550 between w' and T' are significant because these fluctuations are approximately 90° out of phase.
 551 If there is no dissipation $\Delta\phi_{w'T'} = 0$, the contributions from heat flux and energy flux in (11)
 552 cancel each other (see Appendix C for details) and $\overline{w'\theta'} = 0$. But $\overline{w'T'}$ can be positive or
 553 negative depending on the direction of wave propagation, according to Equation (10). If there is
 554 dissipation $\Delta\phi_{w'T'} > 0$ as shown by the Boulder, CO observations (Lu et al., 2017b), $\overline{w'\theta'}$ is
 555 negative and again, $\overline{w'T'}$ can be positive or negative depending on the direction of wave
 556 propagation and the value of $\Delta\phi_{w'T'}$. This result differs from that of Walterscheid (1981), who
 557 concluded that dissipating gravity waves must always exhibit a downward sensible heat flux
 558 regardless of the wave propagation direction. Notice also, if $\Delta\phi_{w'T'}$ is negative, which we
 559 speculate may occur if heat sources are present or the wave is amplified, the positive sensible
 560 heat flux would be even larger. Then according to (11), $\overline{w'\theta'}$ could also be positive. This
 561 possibility is discussed in Section 7.3.

562 **5.2. Estimation of K_E and K_H from Gravity Wave Spectrum**

563 The energy flux and K_E can be derived in terms of the joint vertical wavenumber (m) and
 564 intrinsic frequency (ω) spectrum of the gravity wave temperature fluctuations (Liu, 2009;
 565 Gardner, 2018). Equations (5), (6), and (11), which apply to individual gravity waves, are easily
 566 modified to represent the impact of a spectrum of waves by replacing $A_T^2/2$ by
 567 $F_{T'}(m, \omega)dm d\omega/(2\pi)^2$, where $F_{T'}$ is the 2-D (m, ω) -spectrum of the temperature fluctuations,
 568 and integrating over m and ω . The energy flux, or equivalently K_E , is derived in Appendix A by
 569 employing a model spectrum for $F_{T'}$ and assuming that the spectra of upward and downward
 570 propagating waves are identical

$$571 K_E \simeq (1 - 2\alpha_{down})\beta(s, q) \frac{\Gamma_{adf}}{\bar{T}\sqrt{\xi_{inst}}} \left[\frac{var(T')}{(\Gamma_{ad} + \partial\bar{T}/\partial z)^2} \right]^{3/2}, \quad (12)$$

572 where ξ_{inst} is the normalized lapse rate variance, also called the instability parameter (see (A-
 573 9)), α_{down} is the fraction of wave energy that is propagating downward, and β is a dimensionless
 574 parameter that describes the distribution of wave energy versus m and ω (see (A-7)).

$$575 \beta(s, q) = \begin{cases} \frac{2(s+1)}{s} \sqrt{\frac{(s+1)\ln(N/f)}{(s+3)}} (1 - \sqrt{f/N}) \text{ for } q = 2 \\ \frac{(s+1)}{2s} \sqrt{\frac{(s+1)(\sqrt{N/f} - 1)}{(s+3)}} \ln(N/f) \text{ for } q = 3/2 \\ \frac{(s+1)(q-1)}{s(q-3/2)} \sqrt{\frac{(s+1)(q-1)[(N/f)^{2-q} - 1]}{(s+3)(2-q)}} [1 - (f/N)^{q-3/2}] \text{ for } q \neq 2 \text{ or } 3/2 \end{cases} \quad (13)$$

576 The parameters s and q are characteristics of the spectrum model. For this model the 1-D
 577 intrinsic ω -spectrum is proportional to ω^{-q} and the 1-D m -spectrum is proportional to m^s for
 578 $0 \leq m \leq m_*$ and m^{-2q+1} for $m_* \leq m$, where m_* is the characteristic vertical wavenumber given
 579 by (A4). Although observations have shown that these parameters can vary, the nominal values
 580 are usually assumed to be $s = 1$ and $q = 2$. The nominal value $q = 2$ is consistent with the wide
 581 body of measured spectra in the stratosphere and mesosphere, although observations do suggest
 582 that q decreases as the latitude increases (Pfenninger et al., 1999; Allen & Vincent, 1995). The
 583 energy flux is roughly proportional to the mean vertical phase speed of the waves so that for $0 <$
 584 $s < 1$ and $0 < q < 2$, the magnitude of the energy flux is larger, because the spectrum includes
 585 faster, vertically propagating waves, than for $s = 1$ and $q = 2$. It is important to note that this
 586 expression was derived by assuming that the joint vertical wavenumber (m) and temporal

frequency (ω) spectrum of the downward waves is proportional to the spectrum of the upwardly propagating waves, i.e., only the spectrum magnitudes are different. It is clear from equation (12) that if most waves propagate upward ($\alpha_{down} < 0.5$), K_E and the energy flux will be positive (upward). However, K_E can be negative at some altitudes if the majority of the wave energy is propagating downward. This might occur, for example, in a region of strong primary wave dissipation and subsequent strong secondary wave generation.

Similarly, by combining (2) and (11), we obtain

$$K_H \simeq \frac{f}{(\Gamma_{ad} + \partial \bar{T} / \partial z)^2} \frac{1}{(2\pi)^2} \int d\omega \int dm \sin[\Delta\phi_{w'T'}(m, \omega)] \frac{\omega}{f} F_{T'}(m, \omega) = \varepsilon(q) \frac{fVar(T') \overline{\sin(\Delta\phi_{w'T'})}}{(\Gamma_{ad} + \partial \bar{T} / \partial z)^2}, \quad (14)$$

where

$$\varepsilon(q) = \begin{cases} \ln\left(\frac{N}{f}\right) & \text{for } q = 2 \\ \frac{(q-1)}{(2-q)} \left[\left(\frac{N}{f}\right)^{2-q} - 1 \right] & \text{for } q \neq 2 \end{cases} \quad (15)$$

and

$$\overline{\sin(\Delta\phi_{w'T'})} = \exp[-Var(\Delta\phi_{w'T'})/2] \sin(\overline{\Delta\phi_{w'T'}}). \quad (16)$$

Note in (14), $\overline{\sin(\Delta\phi_{w'T'})}$ represents the sample mean, which is computed with respect to the distribution of wave energy versus m and ω . We assume that many statistically independent waves comprise the wave spectrum so that $\Delta\phi_{w'T'}$ is approximately Gaussian distributed, which leads to (16). Since we do not know theoretically how $\Delta\phi_{w'T'}$ varies with m and ω , this is the best that we can do. However, if we can estimate K_H using the observed data, then (14) and (16) can be used to determine the mean phase shift associated with dissipation and other effects. For the Lu et al. (2017b) dataset, the mean phase shift associated with dissipation was $+2.6^\circ$ and the standard deviation was 26.7° , so that $\overline{\sin(\Delta\phi_{w'T'})} \simeq 0.04$. If these wave dissipation statistics apply approximately to the McMurdo dataset, and the waves in the lower thermosphere at McMurdo are experiencing dissipation similar to the waves observed between 85 and 100 km at Boulder, CO, then according to (14) we find that $K_H \simeq 54 \text{ m}^2/\text{s}$ for $q = 2$ and $K_H \simeq 120 \text{ m}^2/\text{s}$ for $q = 3/2$.

614 As we demonstrated for individual waves of the type encountered in the MLT at
 615 McMurdo, it is possible for a spectrum of waves to induce the large positive heat flux observed
 616 at 103 km. If we assume there is no dissipation and $K_H = 0$, then by applying (3) and (12) with
 617 $K_E = \frac{\overline{w'T'}}{\Gamma_{ad} + \partial \bar{T} / \partial z} \approx 580 \text{ m}^2/\text{s}$, we find that $(1 - 2\alpha_{down})\beta(s, q) = 19.8$, which is achieved if
 618 $\alpha_{down} = 0$, $s = 0.37$, and $q = 3/2$. This wave spectrum model exhibits more energy at the
 619 larger vertical wavelengths and higher frequencies than the nominal $s = 1$ and $q = 2$ model,
 620 which increases the mean phase speed leading to a much larger positive heat flux. Conversely, if
 621 we assume a nominal spectrum dominated by upward-propagating waves ($\alpha_{down} = 0$) with $s =$
 622 1 and $q = 2$, then $K_E = 170 \text{ m}^2/\text{s}$ and according to (3), $K_H \approx -410 \text{ m}^2/\text{s}$. Recall that K_H is the
 623 effective wave-induced thermal diffusivity. Although the cumulative motions arising from a
 624 spectrum of waves appear random, in reality each individual wave imparts an organized motion
 625 to the atmosphere. An upward-propagating spectrum of waves imparts an upward Stokes drift to
 626 the atmosphere which can transport constituents and potential temperature against their density
 627 gradients. Thus, for organized wave motions, K_H can be negative. If $K_H = -410 \text{ m}^2/\text{s}$ when
 628 $q = 2$, then $\overline{\Delta\phi_{w'T'}} \approx -18^\circ$, and if $K_H = -306 \text{ m}^2/\text{s}$ when $q = 5/3$, then $\overline{\Delta\phi_{w'T'}} \approx -7.6^\circ$,
 629 according to (14). These additional phase shifts are comparable to the -8.4° phase shift from
 630 90° predicted by (7) for non-dissipating, upward-propagating waves with vertical wavelengths
 631 averaging 20 km, and the $+2.6^\circ$ measured by Lu et al. (2017b) caused by dissipation of the
 632 mesopause region waves they observed at Boulder, CO. These examples demonstrate the
 633 importance of the wave spectral characteristics, including α_{down} , in determining the sensible
 634 heat, potential temperature, and energy fluxes and their associated diffusivities. The large
 635 positive heat flux in the thermosphere is certainly consistent with theory. However, it is not clear
 636 whether this result arises largely because of changes in the wave spectrum or because K_H is
 637 negative due to phase shifts induced by effects like in-situ heat sources or perhaps, wave
 638 amplification. In Section 6 we gain additional insight about K_H and K_E by comparing the
 639 measured Na and sensible heat fluxes with theory.

640 **5.3. Sensible Heat Flux Profile**

641 The strong dissipation of primary gravity waves before reaching the E_{pm} peak around 86
 642 km (see Figure 4 and discussion in Section 3) leads to a phase shift $\Delta\phi_{w'T'} \gg 0$ thus $\phi_w -$

643 $\phi_T \gg 90^\circ$, resulting in the negative (downward) sensible heat flux as observed. The $\overline{w'T'}$
644 negative peak altitude of ~ 84 km is determined by the competition between the phase difference
645 and wave amplitudes in w' and T' , coupled with the strong downwelling in winter at McMurdo.
646 Severe damping (breaking and cascading to turbulence plus deposition of momentum) of primary
647 waves above the E_{pm} peak leads to the generation of secondary gravity waves that propagate
648 both upward and downward (Vadas et al., 2018; Vadas and Becker, 2019). The nearly zero heat
649 flux between 90 and 95 km is a result of the associated upward and downward fluxes balancing
650 each other, coupled with the initial small amplitudes of the secondary waves (as well as
651 surviving primary waves) that are experiencing little dissipation.

652 The upward-propagating mesoscale secondary gravity waves experience little dissipation
653 from 97 to 102 km as indicated by the E_{pm} profile and its inverse scale height in Figure 4.
654 Therefore, the wave amplitudes in w' and T' grow with decreasing atmospheric density while the
655 phase difference $\phi_w - \phi_T$ remains below 90° (due to the negligible additional phase shift
656 $\Delta\phi_{w'T'} \sim 0$), resulting in the increasingly positive sensible heat flux with a peak at ~ 103 km,
657 according to Equation (5). The E_{pm} growth slows down above 103 km, indicating appreciable
658 dissipation of the secondary waves. The additional phase shift $\Delta\phi_{w'T'}$ associated with dissipation
659 becomes increasingly positive, making the phase difference $\phi_w - \phi_T$ approach 90° . Thus, the
660 positive sensible heat flux starts to decrease in magnitude above 103 km as observed. When the
661 secondary waves experience severe damping or breaking (as indicated by the second peak of
662 E_{pm} around 112 km), the phase difference $\phi_w - \phi_T$ will exceed 90° and result in negative
663 (downward) sensible heat flux again. Unfortunately, the current lidar data signal-to-noise ratio
664 (SNR) does not allow the unambiguous determination of $\overline{w'T'}$ above 106 km.

665 Overall, the profiles of $\overline{w'T'}$, E_{pm} , and inverse scale heights along with the variances in
666 Figure 3 convey a coherent story of heat transport in the MLT by primary and secondary gravity
667 waves via multistep vertical coupling. The impact of these waves on the constituent transport is
668 examined in Section 6. Furthermore, wave amplification and heat sources, if any, could also
669 contribute to the positive $\overline{w'T'}$. This possibility is discussed in Section 7.3.

670 **6. Comparison of the Measured Na Flux with Theory**

Atmospheric constituents can be transported vertically by five different mechanisms: 1) advection, 2) molecular diffusion, 3) eddy diffusion by turbulence, 4) atmospheric mixing by non-breaking waves, and 5) chemical transport by waves and turbulence. Our observations of the Na flux only include mechanisms 4) and 5), viz. the effects of wave mixing and chemical transport caused by wave perturbations in Na chemistry. The theoretical expression for the vertical constituent flux of a chemically active species C, induced by non-breaking gravity waves is given by equations (1)–(4) in Gardner et al. (2019) by simply setting the eddy and molecular diffusivities to zero and multiplying the transport velocities by the species density.

$$\overline{w' \rho_C'} = \bar{\rho}_C \frac{\overline{w' \rho_A'}}{\bar{\rho}_A} - \bar{\rho}_C \left(\frac{g}{R \bar{T}} + \frac{1}{\bar{T}} \frac{\partial \bar{T}}{\partial z} + \frac{1}{\bar{\rho}_C} \frac{\partial \bar{\rho}_C}{\partial z} \right) K_{\text{Wave}} + \overline{w' \rho_C'}_{\text{Chemical}} \quad (17)$$

The parameters ρ_A and ρ_C are the atmospheric and constituent number densities. The first term on the right-hand-side of the (16) is the contribution from the vertical Stokes drift imparted to the atmosphere by the gravity waves (e.g., Coy et al., 1986; Walterscheid & Hocking, 1991). The second term is caused by mixing of the atmosphere by the spectrum of non-breaking waves. Although this term has the form of classical diffusion, as discussed below it is fundamentally different than eddy and molecular diffusion. The third term is the chemical flux which arises from wave-induced perturbations in the constituent chemistry that are partially correlated with the vertical wind fluctuations (Gardner & Liu, 2016). $K_{\text{Wave}} = \overline{w' \zeta}$ is the effective wave diffusivity associated with the wave-induced vertical displacement fluctuations, which we denote by ζ (Gardner, 2018). K_{Wave} is also related to the Stokes drift velocity (Gardner et al., 2019) and to K_H and K_E

$$K_{\text{Wave}} = \frac{g}{N^2} \frac{\overline{w' \rho_A'}}{\bar{\rho}_A} = - \frac{g}{N^2} \left(\frac{\overline{w' T'}}{\bar{T}} - \frac{\overline{w' p'}}{\bar{p}} \right) = K_H + \left(\frac{c_p}{R} - 1 \right) K_E. \quad (18)$$

This expression on the right-hand-side of (18) for K_{Wave} is valid provided each individual wave in the spectrum obeys the gravity wave polarization and dispersion relations and $\frac{\text{var}(\rho_A')}{\bar{\rho}_A^2} \sim \frac{\text{var}(T')}{\bar{T}^2} \ll 1$, which is easily satisfied throughout the MLT above McMurdo. By combining (17) and (18), the constituent flux can also be written as

$$\overline{w' \rho_C'} \simeq -\bar{\rho}_C \left(\frac{g}{R \bar{T}} - \frac{g}{c_p \bar{T}} + \frac{1}{\bar{\rho}_C} \frac{\partial \bar{\rho}_C}{\partial z} \right) K_{\text{Wave}} + \overline{w' \rho_C'}_{\text{Chemical}}. \quad (19)$$

697 Although K_{Wave} has units of diffusivity, atmospheric mixing caused by non-breaking
 698 waves is fundamentally different than classical eddy and molecular diffusion because of the
 699 Stokes drift term and the nature of the organized motion induced by waves. The vertical
 700 temperature gradient $\partial\bar{T}/\partial z$ in the classical diffusion term in equation (17) is replaced by
 701 $-g/C_p = -\Gamma_{ad}$ in the wave mixing term in (19). This change can have a significant impact on
 702 the constituent flux profile and our interpretation of K_{Wave} , especially in the thermosphere where
 703 $\partial\bar{T}/\partial z$ is positive but $-g/C_p$ is negative. K_{Wave} arises through the atmospheric mixing induced
 704 by the spectrum of propagating waves, which is different than the mixing associated with the
 705 random velocity fluctuations caused by turbulence or the random thermal motions of
 706 atmospheric molecules. Each wave imparts an organized, non-random motion to the atmosphere
 707 even though the cumulative effect of the wave spectrum appears random. While molecular and
 708 eddy diffusivities are always positive, K_{Wave} can be negative in regions where the wave
 709 spectrum is dominated by downward propagating waves so that the Stokes drift is downward.
 710 And, as pointed out in the previous section, the wave-induced thermal diffusivity K_H , associated
 711 with the potential temperature flux, can also be negative. For this reason, we refer to the
 712 constituent (and heat) transport caused by this non-random wave mixing as wave transport to
 713 distinguish it from eddy transport caused by the random atmospheric mixing imparted by
 714 turbulence.

715 **6.1. Deriving K_{Wave} , K_H , and K_E from Measured Fluxes**

716 The K_{Wave} , K_H , and K_E profiles can be derived in terms of the measured heat and Na
 717 fluxes by combining (3), (18), and (19) as

$$718 \quad K_{Wave} = - \frac{\left(\overline{w' \rho'_C} - \overline{w' \rho'_C}_{\text{Chemical}} \right)}{\bar{\rho}_C \left(\frac{g}{RT} - \frac{g}{C_p T} + \frac{1}{\bar{\rho}_C} \frac{\partial \bar{\rho}_C}{\partial z} \right)} \quad (20a)$$

$$719 \quad K_H = - \left(1 - \frac{R}{C_p} \right) \frac{\overline{w' T'}}{\left(\Gamma_{ad} + \frac{\partial \bar{T}}{\partial z} \right)} + \frac{R}{C_p} K_{Wave} \quad (20b)$$

$$720 \quad K_E = \frac{R}{C_p} \frac{\overline{w' T'}}{\left(\Gamma_{ad} + \partial \bar{T} / \partial z \right)} + \frac{R}{C_p} K_{Wave} \quad (20c)$$

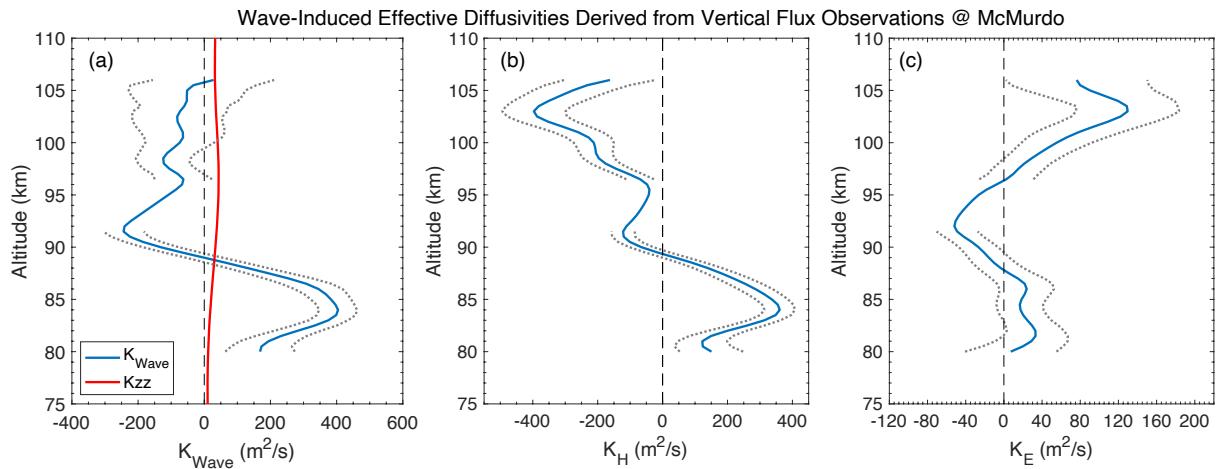
721 Taking into account the measurement uncertainties of Na and heat fluxes, we estimate the
 722 uncertainties of the derived K_{Wave} , K_H , and K_E as

723
$$(\Delta K_{Wave})_{rms} = \frac{(\Delta \overline{w' \rho' Na})_{rms}}{\left| \overline{\rho}_C \left(\frac{g}{RT} - \frac{g}{C_p T} + \frac{1}{\overline{\rho}_C} \frac{\partial \overline{\rho}_C}{\partial z} \right) \right|} \quad (21a)$$

724
$$(\Delta K_H)_{rms} = \sqrt{\left(1 - \frac{R}{C_p}\right)^2 \frac{Var(\Delta \overline{w' T'})}{\left(\Gamma_{ad} + \frac{\partial \bar{T}}{\partial z}\right)^2} + \left(\frac{R}{C_p}\right)^2 Var(\Delta K_{Wave})} \quad (21b)$$

725
$$(\Delta K_E)_{rms} = \sqrt{\left(\frac{R}{C_p}\right)^2 \frac{Var(\Delta \overline{w' T'})}{\left(\Gamma_{ad} + \frac{\partial \bar{T}}{\partial z}\right)^2} + \left(\frac{R}{C_p}\right)^2 Var(\Delta K_{Wave})} \quad (21c)$$

726 To apply the equations in (20), we computed the chemical flux (see Section 6.3 for details) and
727 subtracted it from the measured Na flux profile before deriving the three diffusivities. The
728 denominator of the Na flux term goes to zero near 94 km and the uncertainties become quite
729 large. In this region, we linearly interpolated K_{Wave} and eliminated the error bars on the
730 diffusivity profiles to denote the interpolated region. The profiles of K_{Wave} , K_H , and K_E derived
731 in (20) are plotted, respectively, in Figures 7a, 7b and 7c, along with the eddy diffusivity profile
732 (K_{zz}) obtained from the Whole Atmosphere Community Climate model (WACCM, Wuhu Feng,
733 private communication, University of Leeds).



734
735 *Figure 7. Profiles of (a) the effective wave diffusivity (K_{Wave}), (b) the thermal diffusivity (K_H),*
736 *(c) effectivity diffusivity associated with the gravity wave energy flux (K_E), derived from the*
737 *vertical flux observations in the upper mesosphere and lower thermosphere above McMurdo in*
738 *late May 2020. The red curve in (a) is the eddy diffusivity profile (K_{zz}) obtained from WACCM.*

739 K_{Wave} and K_H exhibit their maximum positive values at 84 km (400 m²/s and 360 m²/s,
740 respectively) where the downward Na and sensible heat fluxes are also maximum (Table 1). This
741 is also the region where wave mixing is large as characterized by the normalized $Var(T')$
742 (Figure 3e) and the atmospheric instability is also large as characterized by the normalized
743 $Var(-\partial T'/\partial z)$ (Figure 3f). K_{Wave} and K_H are negative from 89 to 106 km. As mentioned
744 previously, mixing by non-breaking waves is fundamentally different than mixing by the random
745 turbulence and molecular thermal motions. Waves impart organized motions to the atmosphere
746 which, under certain conditions, can lead to upward potential temperature transport and
747 constituent transport against the concentration gradient. In other words, the wave-induced values
748 of K_{Wave} and K_H can be negative, although in most cases they are expected to be positive. The
749 negative values of K_{Wave} and K_H occur in the mesopause region and lower thermosphere where
750 we have suggested previously that the wave-induced motions may not be strictly adiabatic
751 because of the presence of heat sources and where there may be amplification of some of the
752 gravity waves. Notice that K_E becomes negative in the region between about 88 and 96 km,
753 where the Na flux is positive (upward) and the sensible heat flux is near zero. A negative K_E
754 implies that more than half of the wave energy is propagating downward ($\alpha_{down} > 0.5$, see
755 equation (12)).

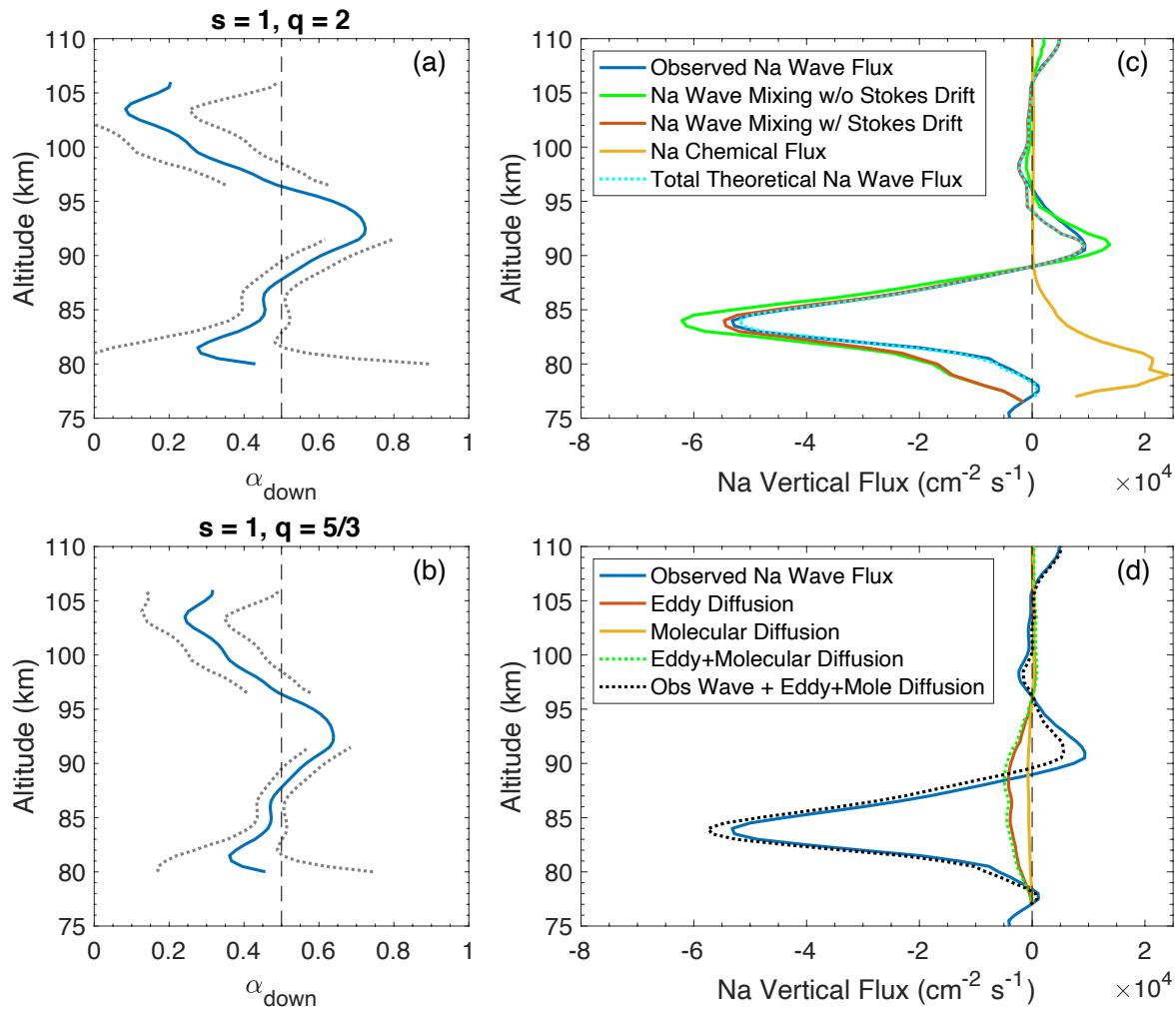
756 **6.2. Estimation and Analysis of α_{down}**

757 Wave dissipation, reflection, and ducting as well as wave sources vary with altitude. All
758 these factors will affect the population of downward propagating waves, making α_{down} altitude
759 dependent. We now apply (12) to gain some insight about α_{down} and the spectrum shape
760 parameters s and q . The factor $(1 - 2\alpha_{down})\beta(s, q)$ can be tuned to produce a theoretical K_E
761 profile given by (12) that closely matches (20c), the profile derived from the measured Na and
762 sensible heat fluxes. We simplify this approach by adopting the nominal values of $s = 1$, $q = 2$,
763 and $\beta(1,2) = 5.8$ at McMurdo and then adjust α_{down} so that (12) equals (20c). Obviously, this
764 approach only provides an estimate of α_{down} because the spectral shape is expected to change
765 with altitude as various waves break, are damped or perhaps are amplified as they propagate
766 through the atmosphere. Because the sign of β is positive, this approach does reveal those
767 regions where more than half the wave energy is propagating downward. The resulting α_{down}
768 profile is plotted in Figure 8a. To illustrate the impact of changes in the wave spectrum with

769 altitude, we also derived the α_{down} profile for $s = 1, q = 5/3$, and $\beta(1,5/3) = 9.356$ and
 770 plotted it in Figure 8b. For $q = 2$, the m -spectrum is proportional to m^{-3} at the highest
 771 wavenumbers and for $q = 5/3$ spectrum is proportional to $m^{-2.33}$. Previous studies have shown
 772 that the m -spectrum does become more shallow in the stratosphere at the higher latitudes
 773 (Pfenninger et al., 1999; Allen & Vincent, 1995). For $q = 2$, α_{down} reaches its maximum value
 774 of 72% at 92.5 km and for $q = 5/3$ the maximum value is 64% also at 92.5 km. Of course, the
 775 α_{down} maxima occur in the region where K_{Wave} was interpolated so the uncertainty is large but
 776 unknown. However, it is clear from the Na flux and transport velocity profiles (Figures 5b and
 777 6b) and equation (19), that K_{Wave} must be negative between 89 and \sim 95 km where
 778 $\left(\frac{g}{RT} - \frac{g}{C_p T} + \frac{1}{\bar{\rho}_{Na}} \frac{\partial \bar{\rho}_{Na}}{\partial z}\right)$ and the Na flux are both positive, while the chemical flux and sensible
 779 heat flux are negligible. From (18) we see that the energy flux must also be negative in this same
 780 region and that requires α_{down} to be larger than 50%. That is, in the region between 89 and 95
 781 km more than 50% of the wave energy must be associated with downward propagating waves,
 782 regardless of the shape of the wave spectrum.

783 Observations and modeling have shown that waves can propagate downward from
 784 sources or reflections at higher altitudes or because the waves are propagating in atmospheric
 785 ducts (e.g., Yu & Hickey, 2007; Walterscheid & Hickey, 2009). Numerous studies, employing
 786 hodograph techniques to unambiguously determine gravity wave propagation directions, have
 787 reported extensive observations of α_{down} made throughout the atmosphere. These studies have
 788 shown that α_{down} can vary over a relatively wide range depending on location, altitude, and
 789 season. For example, Wang et al. (2005) analyzed extensive balloon sonde measurements over
 790 the U.S. and reported that on average \sim 50% of the gravity wave energy propagates downward in
 791 the troposphere and \sim 25% propagates downward in the lower stratosphere. This behavior
 792 suggests that many of the gravity waves may originate in the tropopause region and/or that
 793 waves are being reflected downward in the troposphere. Strelnikova et al. (2020) published
 794 Rayleigh lidar wind measurements made at ALOMAR, Norway (69.3°N, 16.0°E) between 30 and
 795 80 km in the stratosphere and mesosphere. They reported that 32.2% of all the detected gravity
 796 waves propagated downward. By analyzing the middle and upper atmosphere (MU) radar
 797 measurements at Shigaraki, Japan (34.9°N, 139.4°E), Gavrilov et al. (1996) found that 44–51%
 798 of the gravity waves in the altitude range of 70 to 80 km were propagating downward. Hu et al.

799 (2002) employed a Na Doppler lidar to study gravity waves in the mesopause region between 84
 800 and 104 km at SOR (35°N). Only 15.6% of all waves they observed were propagating
 801 downward, while 29% of the shorter vertical wavelength ($\lambda_z < 11 \text{ km}$) waves were propagating
 802 downward. A similar unpublished study was recently conducted with a Na Doppler lidar at Cerro
 803 Pachón, Chile (30°S) where 30.5% of the waves were observed to be propagating downward
 804 (Fabio Vargas, private communication, University of Illinois). Finally, numerical models of the
 805 southern hemisphere MLT developed by Becker and Vadas (2018), suggest that secondary wave
 806 generation is an important process in the mesosphere that can increase the fraction of downward
 807 propagating gravity wave energy. Furthermore, these secondary waves tend to have longer
 808 horizontal and vertical wavelengths than the primary waves from which they are generated
 809 (Vadas et al., 2003, 2018). Therefore, the inferred α_{down} profiles at McMurdo that are plotted in
 810 Figures 8a and 8b are in line with these previous studies and seem plausible.



811

812 *Figure 8. Derived altitude profiles of α_{down} that provide the best match between the measured*
813 *and predicted Na and heat flux profiles for (a) $s=1$, $q=2$ and $\beta(1,2)=5.801$ and for (b) $s=1$,*
814 *$q=5/3$ and $\beta(1,5/3)=9.356$. (c) Comparison of the directly measured and predicted vertical*
815 *fluxes of Na, and (d) comparison of observed wave-induced Na flux with the predicted fluxes*
816 *caused by molecular and eddy diffusion.*

817 **6.3. Predicted Wave Mixing and Chemical Fluxes of Na**

818 The measured Na flux is replotted in Figure 8c along with the wave mixing flux without
819 Stokes drift given by the second term on the right-hand-side of (17) and the wave mixing flux
820 with Stokes drift given by first term on the right-hand-side of (19). In both cases we used the
821 K_{Wave} profile plotted in Figure 7a that was derived according to equation (20a). The Stokes drift
822 velocity is plotted in Figure 6c. Clearly, the upward flux contribution from the Stokes drift at 84
823 km is important as it reduces the magnitude of the maximum downward Na flux so that the
824 predicted Na flux profile caused by wave mixing is in much better agreement with the directly
825 measured profile.

826 The metal layers are formed by meteoric ablation between about 80 and 115 km. Various
827 dynamical processes transport the vaporized atoms and ions downward to chemical sinks below
828 90 km, where they form stable compounds, which then polymerize to form meteoric smoke
829 particles (Plane et al., 2015). The chemical fluxes of the metal atoms are caused by wave-driven
830 perturbations in their chemistry, which induces density fluctuations in the metals that are
831 partially correlated with the vertical wind fluctuations of the waves. Between 80 and 100 km, the
832 chemical loss rate of Na, due to its reaction with O_3 , is significant. However, this reaction
833 produces NaO, which then reacts with O, to quickly recycle the oxide back to Na. Because of
834 this recycling, Na behaves much like an inert species above 90 km, where the meteoric influx is
835 balanced by downward transport to maintain the steady state layer profile. Below 90 km, where
836 the O density decreases rapidly with decreasing altitude, while the atmospheric density and the
837 densities of CO_2 , H_2O , and H_2 increase, this recycling of NaO is inhibited as Na is tied up in the
838 more stable compound $NaHCO_3$. When $NaHCO_3$ forms the dimer or polymerizes with other
839 meteoric constituent molecules, Na is permanently removed from the gas phase (Plane et al.,
840 2015). Above 95 km Na reacts with O_2^+ and NO^+ to form Na^+ via charge transfer and during the
841 day Na can be photoionized. However, during the long polar night in late May at McMurdo,

842 neither of these charge transfer and photoionization processes play a significant role in Na
843 chemistry.

844 The theoretical expression for the chemical flux of Na has been derived by Gardner and
845 Liu (2016) and is given by

846
$$\overline{w' \rho_{Na}'}_{\text{Chemical}} \simeq \left[\frac{(L_{Na} - \mu_{Na})}{\bar{\rho}_{Na}} \frac{\partial \bar{\rho}_{Na}}{\partial z} - \frac{\partial L_{Na}}{\partial z} \right] \frac{\text{Var}(T')}{(\Gamma_{\text{ad}} + \partial \bar{T} / \partial z)^2} \quad (22)$$

847 where μ_{Na} is the meteoric injection rate profile for atomic Na and L_{Na} is the net chemical loss
848 rate profile. Notice that the chemical flux, like E_{pm} and the wave mixing flux (which depends on
849 K_E), depends strongly on the normalized temperature variance plotted in Figure 3e. We compute
850 L_{Na} by assuming that NaHCO_3 is the primary reservoir for Na (Gardner & Liu, 2016; Gardner et
851 al., 2016) and use μ_{Na} derived from the CABMOD ablation model (Carrillo-Sánchez et al.,
852 2020). The net Na loss is computed using the H_2 profile predicted by WACCM, the O_3 , O, H,
853 and H_2O profiles measured by the SABER (Sounding of the Atmosphere using Broadband
854 Emission Radiometry) instrument and the CO_2 profile taken from ACE (Advanced Composition
855 Explorer) as in Beagley et al. (2010). Unfortunately, SABER and ACE observations over
856 McMurdo are only available in late April and late June so those measurements were averaged to
857 estimate the late May profiles needed to compute L_{Na} .

858 To match the observed Na flux, all profiles of these minor species and two major species
859 (N_2 and O_2) were shifted downward by $\Delta z_{down} = 3.5 \text{ km}$. We believe this is justified because
860 the Na density (and Fe density, not shown) and flux profiles are displaced downward by about
861 3.5 km compared to lower latitudes, largely because of the strong downwelling over McMurdo at
862 this time of year caused by the residual circulation system. Because not all the NaHCO_3 is
863 permanently lost and there are uncertainties in some of the reaction rates and species densities,
864 we scaled the loss by 0.5 to obtain the best fit to the observed Na flux. This value is comparable
865 to the 0.57 scaling used by Gardner et al. (2016) to match the Na chemical flux to the
866 observations at SOR.

867 The chemical flux shown in Figure 8c is only significant on the bottomside of the Na
868 layer where it is positive (upward) because $\mu_{Na} < L_{Na}$ and $\partial L_{Na} / \partial z < 0$. The chemical flux of
869 Na peaks near 79 km where it reaches $\sim 2 \times 10^4 \text{ cm}^{-2} \text{s}^{-1}$. When the chemical flux profile is added

870 to the wave mixing flux profile including Stokes drift (see Figure 8c, total theoretical Na wave
871 flux curve), it reduces the negative wave mixing flux near and below 80 km, matching the
872 observed Na flux quite well in this region. Consequently, the total predicted Na flux profile
873 given by equations (17) and (19), is in better agreement with the directly measured Na flux
874 profile at McMurdo than the Na wave mixing flux alone. These results demonstrate that the
875 Stokes drift and chemical flux components make important, non-negligible contributions to the
876 total vertical flux of mesospheric Na induced by non-breaking gravity waves.

877 **6.4. Eddy and Molecular Diffusion Fluxes**

878 Although the McMurdo lidar data were processed in a way that did not include the
879 additional vertical Na flux caused by eddy and molecular diffusion, their effects can be estimated
880 by using the following formula (Gardner et al., 2019)

$$881 \overline{w' \rho_{\text{Na}}'}_{\text{Eddy+Mole}} = -\bar{\rho}_{\text{Na}} \left(\frac{g}{RT} + \frac{1}{T} \frac{\partial \bar{T}}{\partial z} + \frac{1}{\bar{\rho}_{\text{Na}}} \frac{\partial \bar{\rho}_{\text{Na}}}{\partial z} \right) \left[1 + \frac{\text{var}(\partial T'/\partial z)}{(\Gamma_{\text{ad}} + \partial \bar{T}/\partial z)^2} \right] (K_{zz} + K_{\text{Mole}}). \quad (23)$$

882 K_{zz} is the eddy diffusivity generated by breaking waves and K_{Mole} is the molecular diffusivity
883 for Na. This expression is different from the classical formula because the diffusion is enhanced
884 by the normalized lapse rate variance. This enhancement arises because the waves perturb the
885 species mixing ratio gradients, which increases the mixing associated with turbulence and the
886 thermal motion of the Na atoms (Grygalashvyly et al., 2012; Gardner, 2018). The instability
887 parameter, expressed as the normalized lapse rate variance in Figure 3e, is mostly between 0.3
888 and 0.5 but reaches a maximum of 0.7 at 88 km where the environmental lapse rate approaches
889 its largest positive value. Hence, the enhancement of eddy and molecular diffusion, while small,
890 is non-negligible. The Na flux associated with eddy and molecular diffusion was computed by
891 using the K_{zz} profile derived from WACCM simulations and the standard formula for the Na
892 molecular diffusivity (equation (35) in Gardner (2018)). Molecular diffusion of Na is only
893 appreciable at the highest altitudes.

894 The estimated eddy and molecular diffusion fluxes were added to the measured Na flux
895 associated with non-breaking waves and the resulting profile is plotted in Figure 8d. The Na
896 transport velocities induced by molecular and eddy diffusion are compared with the measured
897 wave-induced Na transport in Figure 6d. Although the eddy and molecular Na fluxes and
898 transport velocities are non-negligible, they are much smaller than the wave contributions. This

is not surprising because it has been known for decades that vertical transport induced by propagating gravity waves can be substantial. Walterscheid and Schubert (1989) used a dynamical-chemical model to show that the combined effects of wave dynamics and perturbed chemistry associated with the passage of a gravity wave can result in large downward fluxes of O₃ and OH near 80 km, which alters the mixing ratios of these species and the eddy and molecular diffusion. Hickey et al. (2000) used a 2-D nonlinear model to demonstrate that gravity waves can significantly alter the time averaged atomic O profile in the MLT through the constituent fluxes that the waves induce. Their results showed clearly that the effects of gravity wave transport on the distribution of O in this region can be considerably larger than the effects of eddy transport. Liu and Gardner (2004 & 2005) directly measured the vertical Na flux profiles induced by gravity waves in the MLT using a Na Doppler lidar coupled to large astronomical telescopes at SOR (35°N) and Haleakala, Maui (20°N). Those observations also showed that wave transport of Na was generally much larger than transport by eddy and molecular diffusion.

Despite this early work and the significant heat and Na fluxes reported here, few if any of the global atmospheric chemical models incorporate heat and constituent transport by non-breaking gravity waves, because they cannot resolve the important smaller-scale waves. However, this situation is now changing. Grygalashvyly et al. (2012) employed an effective wave diffusivity, equivalent to the enhanced eddy and molecular diffusivities given by (23), and a numerical model to study the impact of gravity waves on the transport of minor constituents in the MLT. Gardner and Liu (2016) derived generalized theoretical expressions for the chemical fluxes of neutral species induced by waves and turbulence and explored the impact on the transport of O₃, Na, and Fe in the MLT. Gardner et al. (2019) showed how the Stokes drift, chemical fluxes, K_{Wave} , and the enhanced eddy and molecular diffusivities can be derived from most gravity wave parameterizations incorporated in global models. Most recently, Liu (2021) employed the concept of scale invariance to extrapolate the thermal diffusivity (K_H) arising from the large-scale waves resolved by global models, to include the contributions to K_H from the unresolved small-scale waves. This approach could be adapted to also calculate K_{Wave} .

7. Discussion

7.1. Impact of the Complete Temporal Spectrum of Gravity Waves

928 An important characteristic of the McMurdo observations is that the flux measurements
929 represent the contributions from the entire temporal spectrum of gravity waves, while all the
930 previous measurements excluded waves with periods longer than the mean observation periods
931 (~ 6 – 10 h). Guo and Liu (2021) showed that the major contributions to the sensible heat and
932 potential temperature fluxes were made by waves with periods between 5 min and 1 h. The
933 contributions from longer period waves (1–3 h and 3–6 h) were small by comparison. The heat
934 flux measurements at the Starfire Optical Range, Cerro Pachón, and McMurdo are comparable
935 (-2.5 Km/s , see Table 1) and all were made with temporal resolutions sufficient to observe the
936 highest frequency waves with periods as short as the buoyancy period. The heat flux
937 measurements at Hefei were made with a temporal resolution of 10 min, which excludes the
938 highest frequency waves with periods smaller than 20 min and could partially account for the
939 very low heat flux value (-0.3 Kms^{-1}) at this site. The Maui observations also included the
940 highest frequency waves so the lower heat flux value there (-1.4 Kms^{-1}), probably reflects both
941 weaker gravity wave activity at this mid-ocean site and the fact that the Maui value represents
942 the annual mean, not late fall when wave activity should be stronger.

943 Although the Na flux depends in part on the sensible heat flux through K_{Wave} as given by
944 (18), K_{Wave} also has a strong dependence on the total temperature variance through K_E as given
945 by (12). Because the temperature fluctuations have a red frequency spectrum, roughly
946 proportional to ω^{-2} , the longest period waves make the largest contributions to K_E and K_{Wave}
947 and therefore to the Na flux. Only the McMurdo flux observations include contributions from the
948 complete temporal spectrum of gravity waves and in particular, the observations include the
949 persistent inertial-period gravity waves (Chen et al., 2016; Chen & Chu, 2017) that are missing
950 from the other sites. This is important for the constituent fluxes. For example, if we scale the
951 SOR Na flux value in late Nov by the ratio of the Na densities ($\sim 5000/6500$) times the 3/2 power
952 of the ratio of the T' variances ($\sim (110/60)^{3/2}$, to account for the larger values of K_E and K_{Wave} at
953 McMurdo), we obtain $-4.3 \times 10^4 \text{ cm}^{-2} \text{s}^{-1}$, which is comparable to the McMurdo Na flux
954 measurement in late May. Thus, the large McMurdo Na flux appears reasonable and illustrates
955 the important contributions that inertial-period gravity waves make to atmospheric mixing and
956 constituent transport in the MLT.

957 **7.2. Impact of Downward-Propagating Gravity Waves**

958 To match the theoretical Na fluxes with the lidar observations between 89 and 95 km, we
959 inferred that a majority (>50%) of the wave energy was associated with downward-propagating
960 gravity waves. Wave ducting and reflections from above can contribute to downward
961 propagating waves, as well as in-situ wave generation. The similarity of the lidar-observed E_{pm}
962 profile (Figure 4a) to the modeled profile shown in Figure 20 of Vadas and Becker (2019),
963 suggests that the generation of secondary (and tertiary) gravity waves by the body forces
964 produced from the dissipation of primary (and secondary) waves is likely to be a major source of
965 downward propagating waves, especially in the region of 89–95 km where dissipation is
966 significant (Vadas & Becker, 2018 & 2019; Becker & Vadas, 2018; Vadas et al., 2018).
967 Moreover, Joule heating and energetic particle precipitation over McMurdo likely provide extra
968 sources of gravity waves in the lower thermosphere, which would also contribute to the
969 downward-propagating gravity waves at lower altitudes.

970 **7.3. Possible Heat Sources and Wave Amplification in the Lower Thermosphere**

971 McMurdo is located by the edge of auroral oval and polar cap, where energy input from
972 the magnetosphere frequently reaches the bottom of the thermosphere via particle precipitation
973 and Joule heating (e.g., Thayer & Semeter, 2004; Sinnhuber et al., 2012) and the Farley-
974 Buneman instability can also contribute to the heating of the neutral atmosphere (e.g., Dimant &
975 Oppenheim, 2011a, b). Various forms of energy, such as mechanical, chemical, and electrical-
976 magnetic energy as well as solar radiation energy (during daytime), can be converted to the
977 thermal energy of the neutral atmosphere (e.g., Mlynczak & Solomon, 1993; Sinnhuber et al.,
978 2012). Therefore, external heat sources are possible in the lower thermosphere at McMurdo,
979 originating from energy input and forcing from the magnetosphere and ion-neutral coupling,
980 such as Joule heating and energetic particle precipitation, as well as from solar radiation and
981 chemical heating. Indeed, intense aurora emissions at a wavelength of 557.7 nm were observed
982 overhead at McMurdo as well as in the auroral zone during the lidar observation periods with a
983 collocated auroral all-sky camera that was developed by the National Institute of Polar Research
984 (NIPR), Japan and installed at Arrival Heights (Ogawa et al., 2020). An example image of the
985 aurora observations at Arrival Heights on 26 May 2020 is shown in the Supporting Information
986 (Figure S3). The aurora observations provide evidence that heating occurred in the lower
987 thermosphere because the altitude of green-line aurora emissions is usually around 100–120

988 km (e.g., Kurihara et al., 2009). Although McMurdo was in the darkness during the lidar
989 observations, solar energy could be stored and then transported to McMurdo from other sunlit
990 areas and released as chemical heating (Mlynczak & Solomon, 1993).

991 Moreover, lidar observations at McMurdo have demonstrated the super-exponential
992 amplitude growth for tides and planetary waves in the altitude range from 100 to 110 km (Fong
993 et al., 2014, 2015; Lu et al., 2017a). Fong et al. (2014, 2015) reported that the super-exponential
994 growth increases in strength with the K_p magnetic activity index. The tidal results were attributed
995 to a magnetospheric source origin, i.e., in situ generated mainly by polar ionospheric convection
996 and Joule heating (Fong et al., 2015). Lu et al. (2017a) report that the amplitudes of 4-day and
997 2.5-day planetary waves in temperatures also grow rapidly from 1–2 K at 100 km to over 10 K at
998 110 km in May 2014. A seeding-amplification scheme was proposed in Lu et al. (2017a) as the
999 mechanism to amplify surviving 4-day and 2.5-day planetary waves by in situ instabilities. The
1000 positive (upward) sensible heat flux reported here aligns well with these earlier findings in the
1001 lower thermosphere at McMurdo.

1002 Wave dissipation converting wave mechanical (kinetic and potential) energy to thermal
1003 energy can naturally proceed with 100% conversion rate; however, the opposite direction of the
1004 process does not happen easily because of the increase of entropy principle. Nevertheless, wave
1005 amplification converting thermal or other energy into wave mechanical energy can happen,
1006 although it will likely be inefficient and will need some mechanisms (e.g., nonlinearities) to
1007 achieve. A possible scenario could be that localized heating forms pressure differences so
1008 generate large wind shears, leading to instabilities and/or nonlinearities. We speculate that the
1009 instabilities/nonlinearities caused by large wind shears could induce wave amplification and/or
1010 cause negative phase shift between w' and T' , i.e., $\Delta\phi_{w'T'} < 0$, which would lead to positive
1011 sensible heat and potential temperature fluxes. The mechanisms of wave amplification and their
1012 impact on sensible heat and potential temperature fluxes are beyond the scope of this study but
1013 these issues deserve further attention, both theoretically and observationally.

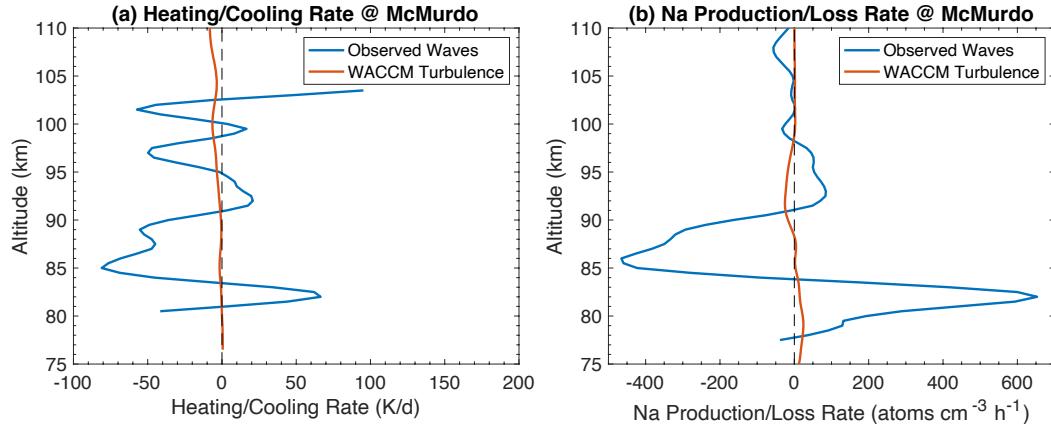
1014 7.4. Wave-driven Heating/Cooling Rate and Na Production/Loss Rate

1015 Examination of the \bar{T} profile reveals that there is a small inversion layer near 85 km with
1016 a full width of about 5 km where the temperature is 5–10 K warmer than the nominal upper
1017 mesospheric profile. This inversion layer may result from local heating caused by gravity waves

1018 dissipating in this region, as well as to the transport of heat downward from above. The heating
1019 rate due to heat flux convergence is

$$1020 -\frac{1}{\bar{\rho}_A} \frac{\partial(\bar{\rho}_A \bar{w}' \bar{T}')}{\partial z} = -\frac{\partial \bar{w}' \bar{T}'}{\partial z} + \left(\frac{g}{R \bar{T}} + \frac{1}{\bar{T}} \frac{\partial \bar{T}}{\partial z} \right) \bar{w}' \bar{T}' . \quad (24)$$

1021 The heating rate profile is plotted in Figure 9a. Also plotted in Figure 9a is the heating/cooling
1022 rate associated with eddy heat transport, which is clearly much smaller compared to the
1023 significant impact of transport caused by non-breaking waves. The heating rate induced by non-
1024 breaking waves approaches nearly 65 Kd^{-1} at 82.5 km while the cooling rate is about
1025 -75 Kd^{-1} at 85 km. The temperature variance reaches a local maximum of 110 K^2 at 85 km
1026 (Figure 3a). In addition, because K_{Wave} is large near 85 km (Figs. 7c and 7f), the fast downward
1027 transport of O into this region will contribute to increased chemical heating associated with the
1028 exothermic reactions involving the excess O. Because the inversion layer is small, the large
1029 heating caused by breaking waves, wave-induced heat transport, and odd-O reactions, must be
1030 balanced by cooling, which could result from wave-transport of CO₂ upward from below. The
1031 CO₂ mixing ratio is relatively constant in the lower mesosphere but exhibits a knee in the profile
1032 near 78 km and falls off above (Beagley et al., 2010). Thus, the enhanced wave mixing
1033 characterized by large K_{Wave} values above 80 km, would increase the upward transport CO₂ into
1034 this region, which in turn would increase the radiative cooling via CO₂ infrared emissions. Of
1035 course, the large values of K_{Wave} are due in part to the relatively large negative vertical gradient
1036 of temperature (i.e., positive environmental lapse rate) associated with the inversion layer which
1037 also affects the values of K_H and K_E as seen in (9)–(11). However, as seen in Figure 7a, K_{Wave} is
1038 negative above 90 km, which would inhibit the downward transport of O in this region, thereby
1039 reducing the impact of chemical heating needed to balance the large cooling rate observed at 97
1040 and 102 km. We acknowledge that this discussion of the influence of gravity waves on the
1041 measured temperature structure at McMurdo is speculative and difficult to reconcile with the
1042 observed heating rate profile. Unfortunately, until models fully incorporate the constituent and
1043 heat transport processes induced by unresolved gravity waves, it will not be possible to obtain a
1044 clear understanding of the precise roles that wave-driven transport plays in the thermal balance
1045 of the MLT.



1046

1047 *Figure 9. (a) Profiles of the heating/cooling rates associated with the convergence of wave-*
 1048 *mixing heat flux and eddy heat flux. (b) Corresponding profiles of the Na production/loss rates*
 1049 *associated with the convergence of Na wave-mixing flux and eddy flux.*

1050 The low 84 km peak in the Na flux is probably caused primarily by the strong
 1051 downwelling over the polar cap in May, but enhanced downward wave transport of Na may also
 1052 play a role. The measured McMurdo Na layer is highly asymmetric with a peak near 88 km,
 1053 which is several km lower than observed at mid-latitudes or even at the South Pole at this time of
 1054 year. The direct effect of vertical constituent transport is local production or loss of the
 1055 constituent. The production/loss rate of Na due to vertical flux convergence is

$$1056 P_{\text{Na}} = - \frac{\partial \overline{w' \rho'_{\text{Na}}}}{\partial z}. \quad (25)$$

1057 The Na production/loss rate profile induced by non-breaking waves is plotted in Figure 9b. The
 1058 Na production rate is about $620 \text{ Na atoms cm}^{-3} \text{ h}^{-1}$ at 82 km. This is balanced by increased
 1059 chemical loss, which is proportional to ρ_{Na} , to maintain the steady-state layer profile. Above 84
 1060 km the production rate is negative, reflecting a loss rate that peaks at about
 1061 $-420 \text{ Na atoms cm}^{-3} \text{ h}^{-1}$ at 86 km. This loss results in a reduction of the Na density in this
 1062 region because the meteoric influx ($\sim 10-20 \text{ cm}^{-3} \text{ h}^{-1}$) does not change. Therefore, the
 1063 transport loss of Na between 84 and 90 km, in combination with the strong wintertime
 1064 downwelling, helps lower the peak of the Na profile to 88 km. For comparison the Na
 1065 production/loss rate associated with eddy transport by turbulence is also plotted in Figure 9b. As
 1066 expected, the impact of eddy transport is small compared to the significant impact of Na
 1067 transport by non-breaking waves.

1068 **8. Conclusions**

1069 The high southern latitude of McMurdo allows continuous long-duration lidar
1070 observations in late May, enabling the coverage of the complete temporal spectrum of gravity
1071 waves from the buoyancy period (~ 5 min) to the inertial period (~ 12.3 h). These Na Doppler
1072 lidar observations, made with high signal-to-noise ratios, coupled with the interleaved data
1073 processing technique, allow the extension of vertical flux and transport measurements upward to
1074 ~ 110 km and downward to ~ 78 km, basically doubling the altitude range of 85–100 km studied
1075 at mid- and low-latitudes. Located by the edge of auroral oval and polar cap where the
1076 downwelling associated with the residual general circulation is strong, the McMurdo lidar
1077 observations have led to several surprising discoveries.

1078 First, the downward Na flux peak is located at 84 km, which is about 4 km lower than
1079 observed at midlatitudes, and the magnitude is double the maximum at midlatitudes. The lower
1080 peak altitude is likely related to the strong downwelling and wave-driven transport over
1081 McMurdo in late May, while the large downward flux is probably related to the enhanced
1082 downward wave transport by the energetic inertial-period gravity waves frequently observed at
1083 McMurdo. This study represents the first-ever flux measurements that include the contributions
1084 from such persistent inertial-period waves and from the complete temporal spectrum of gravity
1085 waves.

1086 Second, to achieve good agreement between the predicted and measured Na flux, we
1087 inferred that in the region between 89 and 95 km, where wave dissipation was significant, a
1088 majority ($>50\%$) of the gravity wave energy was propagating downward. The lidar-observed
1089 profiles of temperature variance and gravity wave potential energy density exhibit two local
1090 maxima around 85 and 112 km, which are quite similar in shape to the E_{pm} profile modeled by
1091 Vadas and Becker (2019) for secondary and tertiary wave generation. We hypothesize that the
1092 large fraction of downward propagating wave energy may be associated with secondary (and
1093 tertiary) waves generated by the dissipation of primary (and secondary) waves, which lends
1094 support to the multistep vertical coupling proposed by Vadas and Becker (2018, 2019).

1095 Third, the measured sensible heat flux exhibits a downward peak at 84 km that is
1096 comparable to the peak values at midlatitudes but lower by about 4 km, while the sensible heat
1097 flux is directed upward (positive) in the lower thermosphere from 97 to 106.5 km. Although we

1098 have focused in this paper on the late May 2020 observations, measurements made on numerous
 1099 other occasions show that positive heat fluxes are common in the lower thermosphere in winter
 1100 above McMurdo. We have shown that the positive sensible heat flux is actually expected from
 1101 the fully compressible polarization relations for non-dissipative gravity waves. Although the
 1102 large positive heat fluxes observed above 100 km could be induced by a suitable spectrum of
 1103 upward-propagating, non-dissipating gravity waves, the observed heat and Na fluxes in this
 1104 region suggest that other factors, such as external heat sources and wave amplification, may also
 1105 play important roles, possibly through affecting the phase shift between w' and T' .

1106 The McMurdo lidar observations illustrate the substantial impact that wave-induced
 1107 transport can have on the temperature and constituent structures of the MLT. These
 1108 measurements show that transport associated with Stokes drift imparted by the gravity wave
 1109 spectrum, chemical transport of reactive species like Na and other meteoric metals, and wave
 1110 transport associated with atmospheric mixing by non-breaking gravity waves, can all make
 1111 significant contributions to constituent and heat transport in the MLT. While this study focused
 1112 on heat and Na transport, wave transport also impacts other important MLT species including O_x ,
 1113 NO_x , HO_x , CO_2 and potentially neutral density and the O/N_2 ratio in the thermosphere, which
 1114 impacts satellite drag. It is now clear that these mechanisms should be incorporated in the next
 1115 generation of global chemistry and general circulation models to fully understand how gravity
 1116 waves influence the structure and composition of the middle and upper atmosphere. Furthermore,
 1117 advanced transport theories and fully compressible polarization relations of gravity waves, which
 1118 account for heat sources and sinks, and for wave dissipation and amplification, should be
 1119 developed in the future.

1120 **Appendix A. Derivation of the Effective Diffusivity Associated with the Energy Flux**

1121 As shown by Liu (2009) and extended by Gardner (2018), the gravity wave polarization
 1122 relations can be used to express the gravity wave energy flux and K_E in terms of the temperature
 1123 fluctuation spectrum as follows

1124
$$K_E = \kappa \frac{g}{N^2} \frac{\overline{w'p'}}{\bar{p}} \simeq \frac{\kappa(1-2\alpha_{down})}{H_p(\Gamma_{ad} + \partial \bar{T} / \partial z)^2} \frac{1}{(2\pi)^2} \int d\omega \int dm \left(1 - \frac{\omega^2}{N^2}\right) \frac{\omega}{m} \frac{m^2 F_{T'}(m, \omega)}{[m^2 + (1-2\kappa\omega^2/N^2)^2/(2H_p)^2]}, \quad (A1)$$

1125 where α_{down} is the fraction of wave energy propagating downward, $F_{T'}(m, \omega)$ is the 2-D power
 1126 spectrum of the wave-induced temperature fluctuations, ω is the intrinsic frequency, and m is the
 1127 vertical wavenumber. The right-hand-side of equation (A1) was derived by assuming that the
 1128 shapes, but not the absolute magnitudes, of the spectra for the upward and downward
 1129 propagating waves are identical, hence the approximately equal sign is used. To evaluate (A1)
 1130 we employ the diffusive filtering theory model spectrum, also used by Gardner (2018), so that

$$1131 \quad F_{T'}(m, \omega) = (2\pi)^2 \frac{Var(T')}{[1-(f/N)^{q-1}]} \frac{(s+1)}{m_*} \left(\frac{m}{m_*}\right)^s \frac{(q-1)}{f} \left(\frac{f}{\omega}\right)^{q+(s+1)/2} \quad m \leq m_*\sqrt{\omega/f}, \quad f \leq \omega \leq N \quad (A2)$$

1132 where m_* is the characteristic vertical wavenumber. Under these conditions the 1-D ω -spectrum
 1133 is proportional to $1/\omega^q$ and the 1-D m -spectrum is proportional $1/m^{2q-1}$ in the region $m_* \leq m$.
 1134 The largest wavenumber $m_*\sqrt{N/f}$ marks the transition from waves to turbulence.

1135 Extensive observations, made at a wide variety of locations and altitudes by many
 1136 different instruments have shown, that the ω - and m -spectra of the horizontal wind and
 1137 temperature fluctuations follow power-laws of the form ω^{-r} , where $r \approx 2$, and m^{-t} in the
 1138 region $m_* < m$, where $t \approx 3$. The model spectrum given by (A2) is consistent with this observed
 1139 behavior for the special case where $q \approx 2$. Furthermore, several theories predict that the m -
 1140 spectrum magnitude remains approximately constant with altitude in the so-called saturation
 1141 regime $m_* < m$, so that as the wave field propagates upward, m_* decreases to accommodate the
 1142 increasing variance of T' . The characteristic vertical wavenumber can be expressed in terms of
 1143 the variance of the lapse rate fluctuations

$$1144 \quad Var(\partial T'/\partial z) = m_*^2 \frac{1}{(2\pi)^2} \int d\omega \int dm \left(\frac{m}{m_*}\right)^2 F_{T'}(m, \omega) = \\ 1145 \quad m_*^2 \frac{Var(T')}{[1-(f/N)^{q-1}]} \frac{(s+1)}{(s+3)} \begin{cases} \ln(N/f) & \text{for } q = 2 \\ \frac{(q-1)}{(2-q)} [(N/f)^{2-q} - 1] & \text{for } q \neq 2 \end{cases} \quad (A3)$$

1146 which yields

$$1147 \quad \frac{1}{m_*^2} = \frac{Var(T')}{Var(\partial T'/\partial z)} \frac{(s+1)}{(s+3)[1-(f/N)^{q-1}]} \begin{cases} \ln(N/f) & \text{for } q = 2 \\ \frac{(q-1)}{(2-q)} [(N/f)^{2-q} - 1] & \text{for } q \neq 2 \end{cases} \quad (A4)$$

1148 K_E can now be computed by substituting (A2) into (A1), neglecting the small
 1149 contributions from terms involving $(\omega/N)^2$, and noting that $1 \ll 2H_p m_*$

1150
$$K_E \simeq \frac{\kappa(1-2\alpha_{down})}{H_p(\Gamma_{ad} + \partial\bar{T}/\partial z)^2} \frac{f}{m_*} \frac{1}{(2\pi)^2} \int d\omega \int dm \frac{\omega}{f} \frac{m_*}{m} F_{T'}(m, \omega) \simeq$$

 1151
$$(1 - 2\alpha_{down}) \frac{\Gamma_{ad} f}{\bar{T} m_*} \frac{var(T')}{(\Gamma_{ad} + \partial\bar{T}/\partial z)^2} \frac{(s+1)(q-1)}{s[1-(f/N)^{q-1}]} \begin{cases} \frac{1-(f/N)^{q-3/2}}{(q-3/2)} & \text{for } q \neq 3/2 \\ \ln(N/f) & \text{for } q = 3/2 \end{cases} \quad (A5)$$

1152 By applying (A4), K_E reduces to

1153
$$K_E \simeq (1 - 2\alpha_{down}) \beta(s, q) \frac{\Gamma_{ad} f}{\bar{T} \sqrt{\xi_{inst}}} \left[\frac{var(T')}{(\Gamma_{ad} + \partial\bar{T}/\partial z)^2 [1-(f/N)^{q-1}]} \right]^{3/2}, \quad (A6)$$

1154 where $[1 - (f/N)^{q-1}] \simeq 1$ for $3/2 \leq q$ and

1155
$$\beta(s, q) = \begin{cases} \frac{2(s+1)}{s} \sqrt{\frac{(s+1)\ln(N/f)}{(s+3)}} (1 - \sqrt{f/N}) & \text{for } q = 2 \\ \frac{(s+1)}{2s} \sqrt{\frac{(s+1)(\sqrt{N/f}-1)}{(s+3)}} \ln(N/f) & \text{for } q = 3/2 \\ \frac{(s+1)(q-1)}{s(q-3/2)} \sqrt{\frac{(s+1)(q-1)[(N/f)^{2-q}-1]}{(s+3)(2-q)}} [1 - (f/N)^{q-3/2}] & \text{for } q \neq 2 \text{ or } 3/2 \end{cases}, \quad (A7)$$

1156 and ξ_{inst} is the normalized lapse rate variance ($Var(\partial T'/\partial z)/(\Gamma_{ad} + \partial\bar{T}/\partial z)^2$) which is also
 1157 called the instability parameter. The normalized lapse rate variance can be expressed in terms of
 1158 Richardson number by expressing the temperature fluctuations in terms of the horizontal wind
 1159 fluctuations by employing the gravity wave polarization relations

1160
$$T' \simeq \frac{N\bar{T}}{g} u'. \quad (A8)$$

1161 After neglecting terms $\partial\bar{T}/\partial z$ and $\partial N/\partial z$, we obtain

1162
$$\xi_{inst} = \frac{Var(\partial T'/\partial z)}{(\Gamma_{ad} + \partial\bar{T}/\partial z)^2} \simeq \frac{Var(\partial u'/\partial z)}{N^2} = \overline{1/Ri}. \quad (A9)$$

1163 $\beta(s, q)$ is tabulated in Table A1 for several values of s and q for McMurdo where the inertial
 1164 period is 12.3 h and the buoyance period is approximately 5 min.

Table A1. $\beta(s, q)$ for $N/f = 148$ at McMurdo

s	q	$\beta(s, q)$
1	2	5.801
1/2	2	8.056
1	5/3	9.356
1/2	5/3	12.99
1	3/2	11.79
1/2	3/2	16.38

1166 **Appendix B. Uncertainties of the Estimated Sample Variances and Fluxes**

1167 The uncertainties of the estimated sample variances and fluxes were derived following
 1168 the approaches described in the appendices of Gardner and Yang (1998) and Gardner and Chu
 1169 (2020). By considering the vertical smoothing associated with the Hamming window, the
 1170 uncertainty associated with estimating the fluctuation variance of the physical variable X from
 1171 the sample covariance function is

$$1172 \Delta Var(X') \simeq \sqrt{2 \frac{L_{X'}}{L_{sm}} \frac{\tau_{X'}}{\tau_{obs}} Var^2(X') + \frac{\Delta z}{L_{sm}} \frac{\Delta t}{\tau_{obs}} [2Var(X')Var(\Delta X) + Var^2(\Delta X)]}. \quad (B1)$$

1173 where prime represents the fluctuations of X and $X' = T', \partial T'/\partial z, w', \rho'_{Na}$. $L_{sm} \simeq 3.42 \text{ km}$ is the
 1174 equivalent rectangular window width of the 5 km full-width Hamming window and $\tau_{obs} = 40 \text{ h}$
 1175 is total observation time. Because the vertical correlation lengths of $T', \frac{\partial T'}{\partial z}$, and ρ'_{Na} are long
 1176 compared to the smoothing interval, for these parameters $L_{X'} = L_{sm}$ and so smoothing does not
 1177 reduce the uncertainty associated with statistical noise. However, vertical smoothing does reduce
 1178 the uncertainty associated with photon noise which is important at the lowest and highest
 1179 altitudes where the Na densities and signal levels are small. For the vertical wind fluctuations,
 1180 which exhibit a nearly white m -spectrum (Gardner & Yang, 1998), $L_{W'} \simeq \Delta z$. The T' spectra
 1181 published by Chen et al. (2016) for the wintertime MLT above McMurdo show that the ω -
 1182 spectra are significantly enhanced near $\omega \simeq 2f$ by the presence of persistent waves with periods
 1183 between ~ 3 and ~ 10 h. This enhancement also distorts the spectral slopes at higher frequencies
 1184 making them steeper. We considered the impact of these persistent waves by modeling the T' ω -
 1185 spectrum as proportional to ω for $f \leq \omega \leq 2f$ and proportional ω^{-2} for $2f \leq \omega \leq N$. For this

model, we computed $\tau_{T'} = \tau_{Na'} \simeq 1 \text{ h}$. Although the persistent waves will also impact the lapse rate spectra, the effects are minor and so we used the correlation time (15 min) derived in Gardner and Chu (2020). The vertical wind ω -spectrum is approximately white so that $\tau_{w'} \simeq 2.5 \text{ min}$.

1190 The uncertainty associated with estimating the vertical flux of the physical variable X
1191 from the sample covariance between the vertical wind and the physical variable (T' or ρ'_{Na})
1192 fluctuations is

1196 The vertical correlation length and correlation times for fluxes are determined by the vertical
 1197 wind so that $L_{w'X'} \simeq \Delta z$ and $\tau_{w'X'} \simeq \Delta t$. The factor of 1/2 in (B2) arises because we derived
 1198 two estimates of the vertical fluxes from the two interleaved w' and X' time series and averaged
 1199 them. The photon noise components contaminating the two flux estimates are statistically
 1200 independent, while the statistical noise components are identical.

1201 The above uncertainties, derived under the assumption of stationary ergodic random
 1202 processes, include contributions from the statistical noise associated with the calculation of the
 1203 sample covariances and fluxes (i.e., the $Var^2(X')$ and $Var(w')Var(X')$ terms) and from the
 1204 photon noise associated with the Poisson distribution of photon counting (i.e., the $Var^2(\Delta X)$ and
 1205 $Var(\Delta X)$ terms). The equations used to estimate the rms uncertainties for the measured variances
 1206 and fluxes in this study are listed in Table B1.

1207 **Table B1. RMS Uncertainties of the Estimated Variances and Fluxes for McMurdo Observations***

Wave-Driven Temperature Variance: $\tau_{T'} \simeq 1 \text{ h}$, $\Delta t = 2.5 \text{ min}$, $\tau_{obs} \simeq 40 \text{ h}$, $L_{T'} \simeq L_{\text{sm}} \simeq 3.42 \text{ km}$

$$\Delta \text{Var}(T') \simeq \sqrt{\frac{1}{20} \text{Var}^2(T') + \frac{0.28}{960} [2\text{Var}(T')\text{Var}(\Delta T) + \text{Var}^2(\Delta T)]}$$

Wave-Driven Lapse Rate Variance: $\tau_{\partial T'/\partial z} \simeq 15 \text{ min}$, $\Delta t = 2.5 \text{ min}$, $\tau_{\text{obs}} \simeq 40 \text{ h}$, $L_{\partial T'/\partial z} \simeq L_{\text{sm}} \simeq 3.42 \text{ km}$

$$\Delta \text{Var}(\partial T' / \partial z) \simeq \sqrt{\frac{1}{80} \text{Var}^2(\partial T' / \partial z) + \frac{0.28}{960} [2 \text{Var}(\partial T' / \partial z) \text{Var}(\partial \Delta T / \partial z) + \text{Var}^2(\partial \Delta T / \partial z)]}$$

Wave-Driven Vertical Wind Variance: $\tau_{w'} \simeq 2.5 \text{ min}$, $\Delta t = 2.5 \text{ min}$, $\tau_{obs} \simeq 40 \text{ h}$, $L_{w'} \simeq \Delta z = 0.96 \text{ km}$, $L_{sm} \simeq 3.42 \text{ km}$

$$\Delta \text{Var}(w') \simeq \sqrt{\frac{0.28}{480} \text{Var}^2(w') + \frac{0.28}{960} [2\text{Var}(w')\text{Var}(\Delta w) + \text{Var}^2(\Delta w)]}$$

Wave-Driven Na Density Variance: $\tau_{\rho'_{Na}} \simeq 1 \text{ h}$, $\Delta t = 2.5 \text{ min}$, $\tau_{obs} \simeq 40 \text{ h}$, $L_{\rho'_{Na}} \simeq L_{sm} \simeq 3.42 \text{ km}$

$$\Delta \text{Var}(\rho'_{Na}) \simeq \sqrt{\frac{1}{20} \text{Var}^2(\rho'_{Na}) + \frac{0.28}{960} [2\text{Var}(\rho'_{Na})\text{Var}(\Delta \rho_{Na}) + \text{Var}^2(\Delta \rho_{Na})]}$$

Wave-Driven Sensible Heat Flux: $\tau_{w'T'} \simeq 2.5 \text{ min}$, $\Delta t = 2.5 \text{ min}$, $\tau_{obs} \simeq 40 \text{ h}$, $L_{w'T'} \simeq \Delta z = 0.96 \text{ km}$, $L_{sm} \simeq 3.42 \text{ km}$

$$\Delta(\overline{w'T'}) \simeq \sqrt{\frac{0.28}{960} \text{Var}(w')\text{Var}(T') + \frac{0.28}{1920} [\text{Var}(w')\text{Var}(\Delta T) + \text{Var}(\Delta w)\text{Var}(T') + \text{Var}(\Delta w)\text{Var}(\Delta T)]}$$

Wave-Driven Na Flux: $\tau_{w'\rho'_{Na}} \simeq 2.5 \text{ min}$, $\Delta t = 2.5 \text{ min}$, $\tau_{obs} \simeq 40 \text{ h}$, $L_{w'\rho'_{Na}} \simeq \Delta z = 0.96 \text{ km}$, $L_{sm} \simeq 3.42 \text{ km}$

$$\Delta(\overline{w'\rho'_{Na}}) \simeq \sqrt{\frac{0.28}{960} \text{Var}(w')\text{Var}(\rho'_{Na}) + \frac{0.28}{1920} [\text{Var}(w')\text{Var}(\Delta \rho_{Na}) + \text{Var}(\Delta w)\text{Var}(\rho'_{Na}) + \text{Var}(\Delta w)\text{Var}(\Delta \rho_{Na})]}$$

1208 * $\text{Var}(X')$ is obtained from the interleaved method while $\text{Var}(\Delta X)$ is 2 times the difference between the total and
1209 wave-driven variances (Gardner & Chu, 2020).

1210 **Appendix C. Heat and Energy Fluxes for Compressible Gravity Waves**

1211 To characterize the sensible heat flux contributed by an individual wave, we employ an
1212 idealized model for the vertical wind and temperature fluctuations induced by a wave of ground-
1213 based frequency ω_r , intrinsic frequency ω , and vertical wavenumber m

1214 $w'(t) = A_w \cos(\omega_r t - mz - \phi_w)$ (C-1)

1215 $T'(t) = A_T \cos(\omega_r t - mz - \phi_T)$ (C-2)

1216 where A_w and A_T are the wave amplitudes, ϕ_w and ϕ_T are the phases for the maximum
1217 fluctuations, and t and z are time and altitude, respectively. The sensible heat flux induced by the
1218 wave is calculated by averaging the product $w'(t)T'(t)$ over the wave period (denoted by the
1219 overbar),

1220 $\overline{w'(t)T'(t)} = \frac{1}{2} A_w A_T \cos(\phi_w - \phi_T)$ (C-3)

1221 The compressible, f-plane, non-dissipative polarization relation for $w'(t)$ and $T'(t)$ is
1222 given by (B-11) in Vadas (2013), which can be written as

1223 $w' = \frac{-ig\omega}{N^2} \frac{\left[1 - \frac{i}{mH} \left(\frac{1}{2} - \frac{1}{\gamma}\right)\right]}{\left[1 + \frac{i}{mH} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2}\right)\right]} \frac{T'}{\bar{T}} = \frac{g\omega}{N^2} \frac{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{1}{\gamma}\right)^2\right]^{1/2}}{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2}\right)^2\right]^{1/2}} e^{-i(\phi_w - \phi_T) \frac{T'}{\bar{T}}}, \quad (C-4)$

1224
1225 where m is negative for upward propagating waves, $\gamma = C_p/C_v \approx 1.4$ for $z \sim 100 \text{ km}$, and the
1226 phase difference between $w'(t)$ and $T'(t)$ is

1227 $\phi_w - \phi_T = \frac{\pi}{2} + \tan^{-1} \left[\frac{1}{mH} \left(\frac{1}{2} - \frac{1}{\gamma} \right) \right] + \tan^{-1} \left[\frac{1}{mH} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2} \right) \right]. \quad (C-5)$

1228
1229 Note that in applying the Vadas (2013) polarization relations, we make the reasonable
1230 assumption that the hatted quantities at a fixed altitude may be replaced by primed quantities.
1231 The sensible heat flux for this single wave is obtained by substituting (C-4) and (C-5) into (C-3)
1232 to compute the cross correlation between w' and T'

1233 $\overline{w'(t)T'(t)} = -\frac{(\gamma-1)}{2\gamma H} \frac{g}{N^2} \frac{A_T^2}{\bar{T}} \frac{\frac{\omega}{m} \left(1 - \frac{\omega^2}{N^2}\right)}{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{(\gamma-1)\omega^2}{\gamma N^2}\right)^2\right]} \simeq -\frac{1}{2} \frac{g^2 A_T^2}{c_p N^2 \bar{T}^2} \frac{\omega}{m} \simeq -\frac{A_T^2}{2\bar{T}} \frac{\omega}{m}, \quad (C-6)$

1234 where the right-hand-side was approximated by assuming $\omega^2 \ll N^2$, $\partial T/\partial z \ll \Gamma_{ad} = g/C_p$, and
1235 $1 \ll 2(mH)^2$. Gravity waves with fast vertical phase speeds and relatively large temperature
1236 amplitudes or with relatively slow vertical phase speeds but very large temperature amplitudes,
1237 can induce large positive sensible heat fluxes. These waves are relatively common in the lower
1238 thermosphere at McMurdo (e.g., Chu, Yu, et al., 2011; Chen et al., 2016), and their predicted
1239 phase shift between w' and T' to values $6 - 10^\circ$ less than 90° can lead to large, positive sensible
1240 heat fluxes induced by upward-propagating, non-dissipating waves, as we observed.

1241 The energy flux for an idealized individual wave can also be derived using the
1242 polarization relation given by (B-7) in Vadas (2013),

1243 $\frac{p'}{\bar{\rho}} = \frac{ig}{m} \frac{\left(1 - \frac{\omega^2}{N^2}\right)}{\left[1 + \frac{i}{mH} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2}\right)\right]} \frac{T'}{\bar{T}} = \frac{g}{m} \left(1 - \frac{\omega^2}{N^2}\right) \frac{\exp[-i(\phi_p - \phi_T)]}{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2}\right)^2\right]^{1/2}} \frac{T'}{\bar{T}}, \quad (C-7)$

1244 where p' is the pressure fluctuation induced by the wave, $\bar{\rho}$ is the mean background density, and
1245 $\phi_p - \phi_T = -\frac{\pi}{2} + \tan^{-1} \left[\frac{1}{mH} \left(\frac{1}{2} - \frac{\gamma-1}{\gamma} \frac{\omega^2}{N^2} \right) \right]. \quad (C-8)$

1246 By computing the cross correlation between w' and p' we obtain

1247 $\overline{w'(t)p'(t)} = \frac{1}{2} A_w A_p \cos(\phi_w - \phi_p) = -\frac{\bar{\rho} g^2}{2N^2} \frac{A_T^2}{\bar{T}^2} \frac{\frac{\omega}{m} \left(1 - \frac{\omega^2}{N^2}\right)}{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{(\gamma-1)\omega^2}{\gamma N^2}\right)^2\right]} \quad (C-9)$

1248 where A_p is the amplitude of the pressure fluctuation, and

1249
$$\phi_w - \phi_p = \pi + \tan^{-1} \left[\frac{(\gamma-2)}{2\gamma m H} \right]. \quad (C-10)$$

1250 Like the heat flux, the energy flux is upward (positive) for upward propagating waves for which
1251 m is negative.

1252 Lu et al. (2017b) measured the phase difference between w' and T' for 184 mesoscale
1253 waves observed between 85 and 100 km at Table Mt., CO. They found that the mean phase
1254 difference $\phi_w - \phi_T = 84.2^\circ$ was 2.6° larger than the phase difference of 81.6° predicted by (C-
1255 5), which they conjectured was likely caused by dissipation associated with damping by eddy
1256 and molecular viscosity. Therefore, to compute the potential temperature θ flux, we add
1257 additional phase small shifts $\Delta\phi_{w'T'}$ and $\Delta\phi_{w'p'}$ to the phase differences between w' and T' and
1258 between w' and p' to account for dissipation. In this case the exact potential temperature flux is

1259
$$\frac{\overline{w'\theta'}}{\bar{\theta}} = \frac{\overline{w'T'}}{\bar{T}} - \kappa \frac{\overline{w'p'}}{\bar{p}} = -\frac{\kappa}{2H} \frac{g}{T^2} \frac{A_T^2 \frac{\omega}{m} \left(1 - \frac{\omega^2}{N^2}\right) [\cos(\Delta\phi_{w'T'}) - \cos(\Delta\phi_{w'p'})]}{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{(\gamma-1)\omega^2}{N^2}\right)^2\right]} -$$

1260
$$\frac{g\omega}{2N^2} \frac{A_T^2}{T^2} \frac{\left\{ \left[1 - \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{1}{\gamma}\right) \left(\frac{1}{2} - \frac{(\gamma-1)\omega^2}{N^2}\right) \right] \sin(\Delta\phi_{w'T'}) - 2 \left(1 - \frac{\omega^2}{N^2}\right) \frac{(\gamma-1)(2-\gamma)}{(2\gamma mH)^2} \sin(\Delta\phi_{w'p'}) \right\}}{\left[1 + \frac{1}{(mH)^2} \left(\frac{1}{2} - \frac{(\gamma-1)\omega^2}{N^2}\right)^2\right]}. \quad (C-11)$$

1261 In deriving (C-11) we note that $\bar{p} = \bar{\rho}R\bar{T}$, $H = R\bar{T}/g$, $R = c_p - c_v$, and $\kappa = \frac{(\gamma-1)}{\gamma} = R/C_p$. It is
1262 easier to interpret $\overline{w'\theta'}$ if we simplify (C-11) by noting that for weak dissipation $\Delta\phi_{w'T'}$ and
1263 $\Delta\phi_{w'p'}$ are only a few degrees (Lu et al., 2017b) and we consider the case where $1 \ll (mH)^2$.
1264 Under these conditions the potential temperature flux reduces to

1265
$$\overline{w'\theta'} \simeq -\frac{g\omega\bar{\theta}}{2N^2} \frac{A_T^2}{T^2} \sin(\Delta\phi_{w'T'}). \quad (C-12)$$

1266 The small phase shifts between w' and p' caused by dissipation and compressibility are
1267 negligible because these fluctuations are nearly 180° out of phase. In contrast, the small phase
1268 shifts between w' and T' are significant because these fluctuations are approximately 90° out of
1269 phase. If there is no dissipation $\Delta\phi_{w'T'} = 0$ and $\Delta\phi_{w'p'} = 0$, the contributions to $\overline{w'\theta'}$ from the
1270 heat and energy fluxes cancel each other and according to (C-11) and (C-12), $\overline{w'\theta'} = 0$.

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1287 **Open Research** The data shown in this work can be downloaded in MatLab data format from
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