Effective vertical diffusion by atmospheric gravity waves

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Abstract

Quantification of heat and constituent transport by gravity waves in global models is challenging due to limited model resolutions. Current parameterization schemes suffer from over-simplification and often underestimate the transport rate. In this study, a new approach is explored to quantify the effective vertical eddy diffusion by using a high-resolution WACCM simulation based on scale invariance. The WACCM simulation can partially resolve the mesoscale gravity wave spectrum down to ~250 km horizontal wavelength, and the heat flux and the effective vertical eddy diffusion by these waves are calculated directly. The effective vertical diffusion by the smaller-scale, unresolved waves, is then deduced based on scale invariance, following the method outlined by Liu (2019) in quantifying gravity wave momentum flux and forcing. The effective vertical diffusion obtained is generally larger than that obtained from parameterizations, and is comparable with that derived from observations in the mesosphere and lower thermosphere region.

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Key Points:

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- Vertical heat flux follows scale invariance with a shallow spectrum.
- Effective vertical diffusion by resolved and unresolved waves are calculated using scale invariance.
- The diffusion coefficient is comparable with values obtained from observations.

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10 Abstract

Quantification of heat and constituent transport by gravity waves in global models is chal-11 lenging due to limited model resolutions. Current parameterization schemes suffer from 12 over-simplification and often underestimate the transport rate. In this study, a new ap-13 proach is explored to quantify the effective vertical eddy diffusion by using a high-resolution 14 WACCM simulation based on scale invariance. The WACCM simulation can partially 15 resolve the mesoscale gravity wave spectrum down to 250 km horizontal wavelength, and 16 the heat flux and the effective vertical eddy diffusion by these waves are calculated di-17 rectly. The effective vertical diffusion by the smaller-scale, unresolved waves, is then de-18 duced based on scale invariance, following the method outlined by Liu (2019) in quan-19 tifying gravity wave momentum flux and forcing. The effective vertical diffusion obtained 20 is generally larger than that obtained from parameterizations, and is comparable with 21 that derived from observations in the mesosphere and lower thermosphere region. 22

²³ Plain Language Summary

Atmospheric gravity waves may transport heat and chemical species in the verti-24 cal direction. Such transport, often measured in terms of an effective diffusion over the 25 large-scale background atmosphere, can be important in controlling the exchange of en-26 ergy and mass between the lower and upper atmosphere, but quantification of the trans-27 port process is challenging because gravity waves are not well resolved or not resolved 28 at all in global models. Previous formulation to approximate the transport tends to over-29 simplify the process, and can lead to model biases. In high resolution models, the larger 30 scale part of the gravity waves are resolved and the transport by these waves can be di-31 rectly calculated from simulation results. This study shows that the transport flux of heat 32 follows scale invariance-a statistical similarity over scales-within the resolved mesoscale 33 range. This scale invariance is used to derive the transport flux by the unresolved waves. 34 It is shown that the transport by the unresolved waves can contribute significantly to 35 the total wave transport. The effective diffusion coefficient derived from this study is com-36 parable to values obtained from observations. 37

38 1 Introduction

Gravity waves (GWs) play a critical role in transporting momentum, heat and con-39 stituents throughout the atmosphere. Their effects need to be parameterized in general 40 circulation models (GCMs), because GWs are a sub-grid scale process (Alexander et al., 41 2010). This was demonstrated as being essential to model the zonal wind reversal and 42 the anomalous winter-to-summer temperature gradient in the mesosphere/mesopause 43 region by Holton (1982, 1983), who used the linear saturation theory (Lindzen, 1981) 44 to parameterize the drag by breaking GWs. It is also shown in later studies that GW 45 drag is important for driving the stratospheric quasi-biennial oscillation (QBO) (Baldwin 46 et al., 2001) and the mesospheric semi-annual oscillation (MSAO) (Dunkerton, 1982; Sassi 47 & Garcia, 1997). 48

GW dissipation is found to induce a net heat flux, which has been determined from 49 a linear theory (Walterscheid, 1981). This is in addition to the diffusion by turbulence 50 induced by GW breaking as formulated in Lindzen (1981). The same idea applies to the 51 transport of constituents, and the wave induced heat/constituent flux has been formu-52 lated in terms of an effective eddy diffusion coefficient (Garcia et al., 2007; A. Z. Liu, 2009; 53 Gardner & Liu, 2010). The formulation by Garcia et al. (2007) is applied in the Whole 54 Atmosphere Community Climate Model (WACCM). Although diffusion from gravity wave 55 breaking is found to play a secondary role in tracer transport in comparison to advec-56 tion (Holton & Schoeberl, 1988), WACCM simulations by Garcia et al. (2014) demon-57 strated that the CO_2 distribution above ~80 km depends sensitively on the effective eddy 58 diffusion coefficient. Furthermore, the values from WACCM (~ 5 to 50 m²s⁻¹ between 59

80–100 km) are found to be smaller than those determined from observations (Swenson et al., 2019), and those required for achieving agreement with various measurements of constituents (Feng et al., 2013; Garcia et al., 2014; Randall et al., 2015; Orsolini et al., 2017; Smith-Johnsen et al., 2018).

Beyond monochromatic wave consideration, Walterscheid and Hocking (1991) suggested that the superposition of a random set of GWs may result in significant parcel dispersion and vertical diffusion in the mesosphere and lower thermosphere (MLT), based on a quasi-linear theory and parcel trajectory simulations. The same study also suggests that the eddy diffusion coefficient obtained from wave flux calculation can oscillate between large down-gradient (positive) and counter-gradient (negative) values.

The combined effects of superposition of transient, finite amplitude, and dissipat-70 ing GWs associated with a myriad of wave sources are not tractable analytically and thus 71 not easily parameterized. Modeling study by GCMs, on the other hand, also faces its 72 own challenges. The foremost challenge is the forbidding cost of simulating the full range 73 of mesoscale GWs, including the wave sources, wave propagation, and wave dissipation 74 in the whole atmosphere environment. It is, however, possible for whole atmosphere mod-75 els to partially resolve the GW spectrum with the current computing power down to sev-76 eral hundred km (e.g., H.-L. Liu et al. (2014); Becker and Vadas (2018)). Effective eddy 77 diffusion coefficient has been calculated for the resolved waves (Grygalashvyly et al., 2012). 78 Large effective diffusion has also been suggested based on scaling argument using high-79 resolution WACCM results (H.-L. Liu, 2017). The challenge for such modeling study is 80 how to maintain the physical consistency between the resolved and parameterized GW 81 effects (the gray zone challenge, (Vosper et al., 2016; H.-L. Liu, 2019)). A strategy to 82 address this challenge is to deduce the effect by unresolved waves from the resolved wave 83 effect based on scale invariance (H.-L. Liu, 2019). This method has been used to calcu-84 late the vertical flux of the GW horizontal momentum and the associated zonal forcing 85 (H.-L. Liu, 2019). In this study, this method is applied to the calculation of vertical eddy 86 diffusion by GWs. 87

⁸⁸ 2 Numerical Model

A high-resolution version of WACCM is used in this study. Detailed description 89 of the model and simulations is found in H.-L. Liu et al. (2014) (and references therein). 90 A brief summary is provided here. WACCM is one of the atmosphere components of the 91 NCAR Community Earth System Model (CESM), with the vertical domain extending 92 to 5.9×10^{-6} hPa (~145 km). The spectral element (SE) dynamical core is used in this 93 study. It is based on a cubed-sphere, with a quasi-uniform horizontal resolution of ${\sim}25$ 94 km and a 0.1 scale height vertical resolution above 40hPa (and higher below). A July 95 simulation with parameterized wave drag (H.-L. Liu, 2017, 2019) is used for the current 96 study. The gravity wave parameterization scheme used in the standard WACCM con-97 figuration (Richter et al., 2010) has been adjusted (H.-L. Liu, 2017) to obtain realistic 98 mean wind and temperature structures. 99

100 3 Analysis

We first examine the zonal wavenumber power spectra of potential temperature θ 101 and vertical wind w and their co-spectrum-the spectrum of vertical heat flux. From Fig-102 ure 1(a), it is seen that the power spectrum of θ ($P_{\theta}(k)$, k is the zonal wavenumber) fol-103 lows a power-law distribution between zonal wavenumber 10 and 100, with a slope of -104 1.9. This is similar to the power spectrum of potential temperature found in the tropo-105 sphere (Nastrom & Gage, 1985). The power spectrum of the vertical wind $(P_w(k))$ fol-106 lows a power-law with a much shallower slope (-0.7), as noted in previous studies (Bacmeister 107 et al., 1996; Lane & Knievel, 2005; Lane & Moncrieff, 2008; H.-L. Liu, 2019). As in the 108 case of the vertical momentum flux (H.-L. Liu, 2019), the shallow slope of the vertical 109

wind leads to a shallow spectrum of vertical heat flux. As seen in Figure 1(c): the ver-110 tical heat flux spectrum $(S_{w\theta}(k))$ has a slope of -1.3, which is the average value of the 111 slopes of $P_{\theta}(k)$ and $P_{w}(k)$. Similar spectral features are found at other altitudes and lat-112 itudes, and Figures 1 (d-f) show the latitudinal dependence of spectral slopes of $P_{\theta}(k)$, 113 $P_w(k)$, and $S_{w\theta}(k)$ at stratospheric, mesospheric and lower thermospheric altitudes (30, 114 75, and 90 km, respectively), with the slope calculated using a method described in H.-115 L. Liu (2019). The latitudinal and height dependence of the spectral slope of $S_{w\theta}(k)$ are 116 very similar to those of the vertical momentum flux (Figure 1 of H.-L. Liu (2019)): the 117 spectral slope variability is larger at lower altitudes, and the largest deviation from the 118 nominal "mean" value (downslope of 7/6) is found at southern (winter) stratosphere and 119 lower mesosphere (below ~ 70 km), likely resulting from the "run-away" jet therein due 120 to missing gravity wave forcing. 121

It is noted that the full spectrum of heat flux $S_{w\theta}(k)$ has both upward (positive) and downward (negative) values, corresponding to counter-gradient and down-gradient fluxes, respectively, with respect to zonal mean potential temperature $(\overline{\theta})$. Overall the down-gradient flux is larger than the counter-gradient flux, as expected, and the spectral components of the counter-gradient fluxes may result from flow transience, nonlinearity, and its spectral transform. In Figure 1(c-f), only the down-gradient components and their slopes are plotted.

An effective vertical eddy diffusion coefficient, in the zonal mean sense, can be calculated from the heat flux and the vertical gradient of zonal mean potential temperature

$$K_{zz} = -\overline{w'\theta'}/(\partial\overline{\theta}/\partial z) \tag{1}$$

with primes denoting perturbation around zonal mean. Here we will focus on the contribution from gravity waves, and the flux term can be calculated from spectral integration between the cutoff zonal wavenumbers on the low and high ends, $k^{<}$ and $k^{>}$, respectively:

$$K_{zz}^{<>} = -\int_{k^{<}}^{k^{>}} S_{w\theta}(k) dk / (\partial \overline{\theta} / \partial z)$$
^(1')

 $k^{<}$ is set to 10 here, and $k^{>}$ should be set to 1000–2000 to cover the full mesoscale range. However, the model can only resolve wavenumber up to $k^{|}$ due to limited model resolution. With a quasi-uniform resolution of ~25 km, the current model can effectively resolve waves with horizontal wavelength of 200 to 250 km. The $k^{|}$ is set to zonal wavenumbers corresponding to wavelength 250 km at each latitude. Part of the total effective eddy diffusion coefficient $K_{zz}^{<>}$ can be directly calculated from the resolved waves, which is denoted as $K_{zz}^{<|}$, using Equation 1' but between wavenumber $k^{<}$ and $k^{|}$. On the other hand, the effective eddy diffusion coefficient from higher wavenumbers, $K_{zz}^{|>}$, cannot be properly accounted for because these waves are unresolved or under-resolved. However, it can be deduced from $K_{zz}^{<|}$ by using scale invariance, like the vertical flux of zonal momentum and zonal forcing (H.-L. Liu, 2019):

$$K_{zz}^{|>}/K_{zz}^{<|} = \begin{cases} ((k_{>}/k_{|})^{1-\alpha} - 1)/(1 - (k_{<}/k_{|})^{1-\alpha}) & \text{if } \alpha \neq 1\\ \ln(k_{>}/k_{|})/\ln(k_{|}/k_{<}) & \text{if } \alpha = 1 \end{cases}$$
(2)

where α is the down-slope value of the spectrum. As noted above, there are wave components with upward heat flux, and the apparent K_{zz} associated with these spectral components would be negative $(K_{zz}(k^-) < 0)$. Both the positive and negative spectral values, $K_{zz}(k^+)$ and $|K_{zz}(k^-)|$, display power-law distribution, though their slopes could be different. The spectral calculation described above is performed separately for the two, and then summed (with sign) to obtain the net K_{zz} .

Figures 2(a-c) show the K_{zz} by the resolved waves $(K_{zz}^{<|})$, by the under-/un-resolved waves deduced from Equation 2 $(K_{zz}^{|>})$, and the sum of the two. The parameterized K_{zz}

is shown in (d) for comparison. $K_{zz}^{<|}$ increases with altitude, from 10^{-3} – 10^{-2} m²s⁻¹ in the lower stratosphere to $\sim 10^2$ m²s⁻¹ in the lower thermosphere. Its latitude-height struc-137 138 ture is similar to that of the zonal forcing by gravity waves (H.-L. Liu, 2019). $K_{zz}^{|>}$ also 139 has a similar spatial structure, and its magnitude is comparable to or even larger than 140 $K_{zz}^{<|}$. $K_{zz}^{|>}$ is over 1000 m²s⁻¹ at high latitudes in the southern stratosphere and lower 141 mesosphere. This is due to the over-flattening of the wave spectra therein, as can be seen 142 from Figure 1(d). For example, the spectral slope is 0 around 50°S at 30 km, and ac-143 cording to Equation 2 $K_{zz}^{|>}$ would be ~10 times larger than $K_{zz}^{<|}$. This over-flattening 144 of the wave spectra is caused by the unrealistically large winter jet, which is in turn due 145 to insufficient gravity wave forcing (H.-L. Liu, 2019). 146

The total $K_{zz}^{<>}$ $(K_{zz}^{<|} + K_{zz}^{|>})$ has similar spatial structure and magnitude to the parameterized K_{zz}^{P} in the mesosphere (70-85 km) (though at SH higher latitudes the former is generally larger). At altitudes below and above $K_{zz}^{<>}$ is larger than K_{zz}^{P} . This is 147 148 149 because the parameterization used is based on the linear saturation theory for wave break-150 ing (Lindzen, 1981), and in WACCM it has been tuned so that much of the wave break-151 ing occurs around MLT to reverse the zonal wind. It is worth noting that the latitude/height 152 structure of K_{zz}^{zz} is in good agreement with that of the absolute momentum flux derived 153 from satellite observations from the stratosphere to the lower thermosphere (Ern et al., 154 2018). $K_{zz}^{\langle \rangle}$ is thus more realistic than K_{zz}^P . 155

Averages globally, over the northern/southern hemispheres (NH/SH) poleward of 30° and over the tropical region of $K_{zz}^{<|}$, $K_{zz}^{|>}$, $K_{zz}^{<>}$, and K_{zz}^{P} are shown in Figure 3(a). The equivalent transport coefficient K_{adv} associated with the residual-mean vertical velocity, \overline{w}^{r} , is calculated as

$$K_{adv} = |\widehat{\overline{w}^r \theta} / \frac{\partial \overline{\theta}}{\partial z}| \tag{3}$$

following Holton and Schoeberl (1988), and its area-weighted averages (hat sign) are shown 156 in respective plots. It is noted that an alternative method is to define K_{adv} as $\left|\overline{w}^r \frac{\partial \theta}{\partial z} \right| \left| \frac{\partial^2 \theta}{\partial z^2} \right|$ 157 since this would apparently facilitate direct comparison of the advective term and the 158 diffusive term. However, $\frac{\partial^2 \overline{\theta}}{\partial z^2}$ is close to 0 at some latitudes and altitudes, making it dif-159 ficult to interpret the result. On the other hand, at altitudes where this second order deriva-160 tive is finite, the transport coefficients calculated from the two methods are found to be 161 comparable. The mean molecular diffusion is also plotted for comparison. By compar-162 ing the global mean of $K_{zz}^{<|}$ and $K_{zz}^{|>}$, it is seen that the two are comparable between $\sim 70-$ 163 95 km, and the latter (diffusion by unresolved waves) is larger/smaller at lower/higher 164 altitudes. As discussed earlier, $K_{zz}^{|z|}$ becomes extremely large in the southern stratosphere 165 and lower mesosphere at higher latitudes, where the wave spectra become excessively flat. 166 This is also reflected in the global average. The total K_{zz} and K_{zz}^{P} are comparable at 167 75 to 80 km. At lower altitudes, K_{zz}^P is 2–3 orders of magnitude less than the total K_{zz} , 168 and is actually similar to the molecular diffusion between 20 and 50 km. K_{zz}^P also de-169 creases rather quickly with altitude above 75 km, and crosses the molecular diffusion co-170 efficient profile at 90 km. The homopause height according to K_{zz}^P is thus 15–20 km too 171 low compared with the accepted value (105–110 km) (Schunk & Nagy, 2009; Andrews 172 et al., 1987). On the other hand, the total K_{zz} increases with altitude above 70 km, and 173 becomes equal to the molecular diffusion coefficient profile at 103 km. In comparison with 174 K_{adv} , the total K_{zz} is less at all altitudes below 100 km, except when it becomes unre-175 alistically large near ~ 50 km. This is consistent with the conclusion reached by Holton 176 and Schoeberl (1988), that the vertical eddy diffusion is in general secondary to advec-177 tive transport. However, hemispheric and latitudinal dependence are noted in the com-178 parison (Figure 3(b-d)): K_{zz} and K_{adv} become more comparable in the winter hemisphere 179 (SH) in the mesosphere and lower thermosphere (especially at higher latitudes). The NH 180 and SH difference in K_{adv} results from the different temperature structure: The tem-181 perature increases with altitude at a faster rate-thus has a shorter vertical scale-in the 182 winter MLT than in the summer, due to the adiabatic heating associated with the down-183

welling driven by gravity wave drive. This result suggests that the vertical diffusion can
 play an important role in the vertical transport in winter time MLT at higher latitudes.

It is found that the total K_{zz} calculated using the method outlined here does not have a sensitive dependence on $k^{|}$. The K_{zz} shown in the figures is obtained by setting $k^{|}$ to zonal wavenumbers corresponding to 250 km zonal wavelength for each latitude. The calculation has been repeated by changing the horizontal wavenumber to 400 km (with the small and large wavenumber cutoffs unchanged), and the total K_{zz} obtained is similar.

$_{192}$ 4 Discussion

The effective diffusion may result from gravity wave dissipation (Walterscheid, 1981) 193 and dispersion by randomly superposed gravity waves (Walterscheid & Hocking, 1991; 194 Lukovich & Shepherd, 2005). Nonlinearity can also lead to apparent transport, but it 195 may not act coherently on the mean flow over time, and considerable cancelation may 196 occur when averaged over time (Walterscheid & Hocking, 1991; Nakamura, 2001). As 197 such, the diffusion coefficient deduced from wave flux calculation (Equation 1) (i) may 198 vary significantly over time, and (ii) is not positive definite. This issue is examined here. 199 As discussed in the previous section, down-gradient and counter-gradient fluxes are sep-200 arated when analyzing the heat flux spectrum, and so are the calculations of the diffu-201 sion coefficients by the resolved and unresolved waves. In Figure 4, the positive and neg-202 ative $K_{zz}^{\langle |}$ and $K_{zz}^{|\rangle}$ and their sums are shown at several altitudes. The values in the NH and the SH are shown separately, since the $K_{zz}^{|\rangle}$ values in the two hemispheres can dif-203 204 fer significantly. It is seen from the figure that at all the altitudes and latitudes the to-205 tal $K_{zz}^{<|}$ and $K_{zz}^{|>}$ are positive, indicating the flux calculation using potential tempera-206 ture can indeed yield the net down-gradient flux. It is also seen that the values of the 207 positive and negative K_{zz} (equivalently the down and counter gradient heat fluxes) are 208 several times larger than the net values. This confirms the findings by Walterscheid and 209 Hocking (1991) that there is considerable cancelation between the two. 210

Figure 4 also shows that the latitudinal dependence of $K_{zz}^{<|}$ and $K_{zz}^{|>}$ can be dif-ferent. For example, at 90 km $K_{zz}^{<|}$ has similar values at the equator and at middle north-ern latitudes (net values between 10–20 m²s⁻¹), but $K_{zz}^{|>}$ values at middle northern lat-211 212 213 itudes is much larger than the equatorial values (over 30 $m^2 s^{-1}$ vs nearly 0). This is be-214 cause of the latitudinal dependence of the spectral slope. As seen from Figure 1(f), at 215 90 km the slope is much flatter at middle northern latitudes (down slope value ~ 0.8) than 216 at the equator (down slope value ~ 1.4). The spectral slopes of the positive and nega-217 tive K_{zz} (down and counter gradient fluxes) can also be different, with the former gen-218 erally flatter than the latter (thus the positive net $K_{zz}^{|>}$ values). 219

The average eddy diffusion coefficient obtained here (Figure 3) is comparable to 220 that deduced from observations in the MLT region. For example, the total K_{zz} shown 221 in Figure 3(a) between 90–95 km is $30-50 \text{ m}^2\text{s}^{-1}$. Salinas et al. (2016) derived eddy dif-222 fusion from SABER CO₂ measurement, and it is $\sim 33 \text{ m}^2 \text{s}^{-1}$ at 90 km. Swenson et al. 223 (2019) obtained global mean eddy diffusion coefficient from O determined by SABER 224 OH measurements, with odd oxygen loss considered, and the value is $33-60 \text{ m}^2 \text{s}^{-1}$ be-225 tween 90–95 km. This is smaller than the eddy diffusion coefficient from an earlier es-226 timate without considering the odd oxygen loss (Swenson et al., 2018). It is also smaller 227 than the mean eddy diffusion coefficient estimated from O determined from SCIAMACHY 228 measurements (70–90 $m^2 s^{-1}$ for the same altitude range). It is worth noting that at 97 229 km, the total K_{zz} from Figure 3(a) is ~60 m²s⁻¹. This is less than the eddy diffusion 230 coefficient applied at the lower boundary of TIE-GCM (~97 km) by Qian et al. (2009), 231 $200-250 \text{ m}^2 \text{s}^{-1}$ around June solstice, to obtain agreement of the thermospheric density 232 between TIE-GCM simulation and that inferred from satellite drag. However, the effec-233 tive diffusion coefficient obtained in that study is a measure of all dynamical effects not 234

included in the model, including large-scale processes such as mean circulation and tidal effects (Jones Jr. et al., 2017). For example, K_{adv} is between 100 and 200 m²s⁻¹ according to Figure 3(a).

As mentioned in the Introduction, previous numerical experiments suggested that 238 the vertical eddy transport in WACCM tends to be too weak. For example, Feng et al. 239 (2013) found from a 1-D model that an effective diffusion coefficient of $\sim 200 \text{ m}^2\text{s}^{-1}$ is 240 needed for 80–90 km at mid-latitude to sustain a meteoric input of more than 20 td^{-1} , 241 while the parameterized K_{zz} from that WACCM version used was 5 m²s⁻¹ and could 242 only sustain a meteoric input of 2.1 td⁻¹. The total K_{zz} from the calculation presented 243 in this study is $\sim 45/30 \text{ m}^2 \text{s}^{-1}$ at 90km and 40°N/S. This is still less than the required 244 value of $\sim 200 \text{ m}^2 \text{s}^{-1}$. However, eddy diffusion is the only transport process considered 245 in the 1-D model, and large-scale dynamics would account for a significant portion of the 246 vertical transport. For example, the transport coefficient corresponding to the downward 247 residual circulation in the winter hemisphere is between $45-80 \text{ m}^2 \text{s}^{-1}$ within the 80-90248 km altitude range (Figure 3(c)). Other studies also found the need to increase the pa-249 rameterized K_{zz} by decreasing the effective Prandtl number (Garcia et al., 2014; Orsolini 250 et al., 2017; Smith-Johnsen et al., 2018). For example, a much better agreement between 251 simulated and observed CO_2 in the MLT can be achieved when the Prandtl number is 252 reduced by half, thus doubling the global mean K_{zz} from 7, 20, and 45 m²s⁻¹ to 14, 40 253 and 90 $m^2 s^{-1}$ at 80, 90 and 100 km, respectively (Garcia et al., 2014). The latter set of 254 values are comparable to the NH averaged values shown in Figure 3. 255

Vertical effective diffusivity (Nakamura, 2001) by gravity waves in the MLT has been 256 computed from numerical experiments using an off-line coupled model of the dynamics 257 and chemistry (Kuehlungsborn Mechanistic general Circulation Model–MEsospheric Chemistry-258 Transport Model, or KMCM-MECTM), both by full dynamical fields from the simula-259 tion and by dynamical fields with the resolved smaller scales (350–1000km) filtered out 260 (Grygalashvyly et al., 2012). The effective diffusion coefficients obtained, which are by 261 waves with the horizontal scales between 350–1000 km, have spatial structures similar 262 to the total K_{zz} in Figure 2, with an upward-poleward tilting mesosphere peak between 263 60-90 km in the NH, a "mixing barrier" layer of ~ 5 km above, and further increases above 264 that. The spatial structure in the winter hemisphere is also similar, except for the very 265 large values found in the stratosphere and lower mesosphere "cold pole" in the current 266 study. The MLT values from that study, however, are much larger than those obtained 267 here, with mesospheric maximum values in the summer hemisphere over $350 \text{ m}^2 \text{s}^{-1}$ at 268 60° latitude between 80-85 km, and maximum in the winter hemisphere at 100 km reach-269 ing 500 $m^2 s^{-1}$ at middle to high latitudes. They are also larger than the values deter-270 mined from observational and parameterization studies mentioned above. The larger val-271 ues would also imply a higher turbopause. The cause of this discrepancy is unclear and 272 needs to be determined in future studies, when atmosphere constituents are included in 273 high-resolution WACCM simulations. 274

²⁷⁵ 5 Summary and Conclusion

The zonal wavenumber spectrum of the vertical heat flux calculated from a highresolution WACCM simulation is shown to follow a power-law distribution in the resolved mesoscale range. The spectral slope varies with latitude and height, and is similar to the slope of the vertical flux of horizontal momentum flux (H.-L. Liu, 2019). They are shallower than the spectral slopes of zonal spectra of kinetic and potential energies, likely due to the flat vertical wind spectrum. The smaller scale waves can thus contribute significantly to the total vertical fluxes.

The vertical eddy diffusion coefficient (K_{zz}) is calculated from the ratio between the vertical heat flux and the vertical gradient of zonal mean potential temperature. The contribution from the resolved gravity waves to K_{zz} (and equivalently the vertical heat

flux), can be directly calculated from the co-spectra of potential temperature and ver-286 tical wind. The contribution by under-resolved and unresolved waves can be deduced 287 from the resolved portion of the spectra based on scale invariance, following the method 288 discussed in H.-L. Liu (2019). The calculation is performed separately for the down-gradient 289 heat flux (positive K_{zz}) and for the counter-gradient flux (negative K_{zz}). The two have 290 large cancellations, and the net heat flux is down-gradient and the total K_{zz} is positive. 291 Eddy diffusion coefficients by smaller scale, unresolved waves are indeed comparable or 292 even larger than that by resolved waves. 293

294 The K_{zz} values are in general agreement with vertical eddy diffusion values deduced from observational and parametric studies. The globally averaged total K_{zz} increases 295 consistently with altitude, and is equal to molecular diffusion at ~ 103 km, consistent with 296 the homopause altitude. This study thus provides a method to directly calculate the ef-297 fective vertical diffusion by gravity waves when the waves are partially resolved by the 298 model. The total K_{zz} thus obtained are generally larger than that from gravity wave pa-299 rameterization, except in the mesosphere where the two become comparable. This is prob-300 ably because the gravity wave parameterization scheme in the model has been tuned to 301 reproduce the wind and temperature structures in the mesosphere/mesopause region. 302 The parameterized K_{zz} is thus likely underestimating the vertical transport in the lower 303 thermosphere, a region critical for controlling atmosphere-geospace mass exchange, as 304 well as the vertical transport below the mesosphere. 305

Figure 1. Zonal wavenumber power spectrum density (PSD) of (a) potential temperature and (b) vertical wind at the equator and 75 km altitude. (c): the zonal wavenumber spectrum of the vertical heat flux at the same location. The thin straight lines in the plots indicate the power-law slope, and the slope values are marked by the lines. Downslope values of the heat flux spectrum (solid line) and PSD of potential energy (dotted line) and vertical wind (dashed line) at (d) 30 km, (e) 75 km and (f) 90 km. These are averages over 7 days (3–9 July).

Figure 2. Effective diffusion coefficient by (a) resolved waves, (b) unresolved waves and (c) the sum of the two. (d): monthly mean parameterized eddy diffusion coefficient for July according to Garcia et al. (2007).

Figure 3. Averages (a) globally, over (b) NH and (d) SH poleward of 30° , and (c) the tropical region of the effective eddy diffusion coefficient by resolved waves (blue dotted line), unresolved waves (blue dashed line), and their sum (blue solid line). In comparison, the black solid line is the molecular diffusion, the red solid line is the parameterized eddy diffusion coefficient, and the black dash-dot line is the equivalent transport coefficient by residual-mean vertical velocity (Equation 3).

Figure 4. The down-gradient (dotted line) and counter-gradient (dashed line) eddy diffusion coefficients and their sum (solid line) by the resolved waves (red) and unresolved waves (navy blue) at (a, b) 30 km, (c, d) 75 km, and (e, f) 90 km, and for the NH (a, c, e) and the SH (b, d, f).

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- ³¹⁴ Systems Laboratory (CISL) at NCAR. NCAR CESM/WACCM is an open-source community model, and is available at https://doi.org/10.5065/D67H1H0V. Model output
- used for this study is available at https://doi.org/10.5065/rxae-ab06.

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Figure 1.

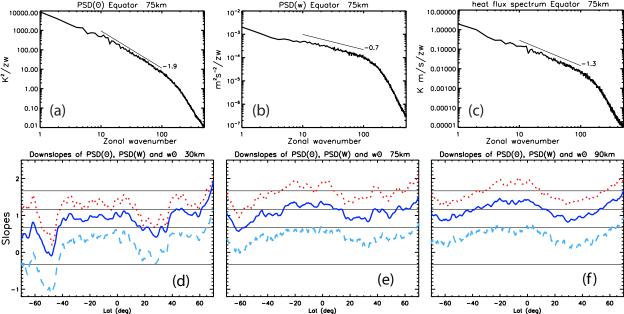


Figure 2.

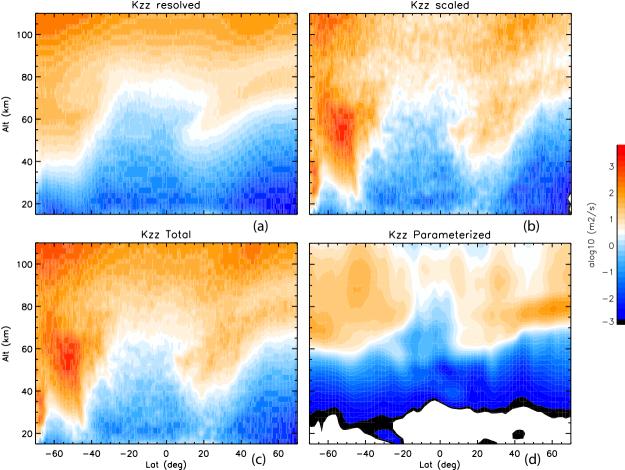


Figure 3.

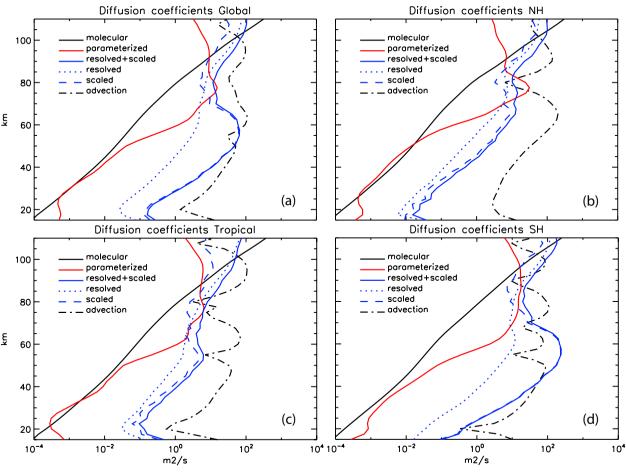


Figure 4.

