A Deep Learning Parameterization of Gravity Wave Drag Coupled to an Atmospheric Global Climate Model

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11	Key Points:
12	• A neural network can accurately and stably emulate a physics-based parameter-
13	ization of gravity wave drag when coupled to a climate model.
14	• When trained on one phase of the quasi-biennial oscillation, the emulator can gen-
15	erate an entire cycle of the quasi-biennial oscillation.
16	• The emulator captures the response of the original gravity wave parameterization
17	to enhanced CO2.

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18 Abstract

19	We present a novel, single-column gravity wave parameterization (GWP) that uses ma-
20	chine learning to emulate a physics-based GWP. An artificial neural network (ANN) is
21	trained with output from an idealized global climate model (GCM). We show that an
22	ANN can learn the distribution of gravity wave drag directly from resolved flow variables.
23	When coupled with a GCM, the ANN generates a quasi-biennial oscillation (QBO) with
24	a realistic amplitude and period and is stable for multidecadal timescales. When forced
25	by increasing concentrations of CO2, the ANN's climatological response is similar to that
26	generated by the physics-based GWP. Finally, we show that the local horizontal wind
27	components are the only essential training features for reasonable emulation and online
28	stability. State-of-the-art GWPs differ in functional form, and are limited in their abil-
29	ity to incorporate observations. This work constitutes a significant step towards obtain-
30	ing observationally validated, computationally efficient GWPs in GCMs.

³¹ Plain Language Summary

Atmospheric gravity waves (GWs) or "buoyancy waves" are generated by pertur-32 bations in a stably-stratified environment. They mediate momentum transport between 33 the lower and middle atmospheres and play a leading-order role in driving middle atmo-34 spheric circulation. Due to computational constraints and a lack of observations, global 35 climate models "parameterize" or estimate the effect of GWs on the large-scale flow. Current climate predictions are sensitive to uncertainties in these representations, partic-37 ularly at the regional scale. Here, we present a novel approach to parameterizing GWs 20 by training a neural network to emulate an existing gravity wave parameterization in a 39 global climate model. This approach represents an appealing technique to build data-40 driven gravity wave schemes that can reduce existing uncertainties. 41

42 1 Introduction

Atmospheric gravity waves (GWs) play an important role in surface climate (Palmer 43 et al., 1986) and a leading-order role in driving middle atmospheric circulation, struc-44 ture, and variability (Fritts & Alexander, 2003). By transporting momentum, GWs im-45 pact the mean climatology (Bretherton, 1969; Sato & Hirano, 2019). They are critical 46 for variability, impacting the jet stream and storm tracks (Fritts & Nastrom, 1992) and 47 stratospheric dynamics (Antonita et al., 2007; Kang et al., 2018; Limpasuvan et al., 2012). 48 Since much of the gravity wave spectrum $(10^1 \text{ to } 10^5 \text{ kilometers})$ is too fine to be cap-49 tured at current model resolutions, models typically mimic its effects on the resolved cir-50 culation via explicit Gravity Wave Parameterizations (GWPs) (Fritts & Alexander, 2003; 51 Richter et al., 2010). 52

Incorporating a realistic representation of these effects in numerical models, how-53 ever, remains challenging for several reasons: i) The absolute magnitude of GW momen-54 tum flux is not well-constrained by observational or intermodel studies (Geller et al., 2013). 55 ii) GWs are generated by a variety of sources, including orography, convection, and fron-56 togenesis (Fritts & Alexander, 2003), but the representation of their sources is not uni-57 form among models. iii) For a given source, the details of the GWP can vary greatly be-58 tween models (Butchart et al., 2018), and even small changes within the same model can 59 lead to diverging regional climate projections (Schirber, 2015). iv) The horizontal prop-60 agation of GWs is usually neglected in parameterizations, which is nonphysical and has 61 an impact on the middle atmosphere (Xu et al., 2017). v) There tends to be a compen-62 sation between resolved and unresolved waves (Cohen et al., 2013), complicating obser-63 vational and intermodel comparisons. 64

Despite these limitations, GWPs can be optimized towards maximizing global fore-65 cast skill scores (Alexander et al., 2019) or "tuned" to reduce climatological biases (Garcia 66 et al., 2017). However, these limitations become apparent in simulations of future cli-67 mate. Projections of the tropospheric and stratospheric circulations' response to anthro-68 pogenic forcing are sensitive to uncertainties in GWPs (Sigmond & Scinocca, 2010; Polichtchouk 69 et al., 2018). Such limitations indicate the need for the continued development of GWPs, 70 preferably with observational validation, computational efficiency, and minimal bias stem-71 ming from underlying physics-based assumptions. 72

An alternative approach to physics-based parameterization has emerged in the form 73 of machine learning (ML). ML has been employed to parameterize processes such as con-74 vection (Rasp et al., 2018; Gentine et al., 2018) and radiation (Brenowitz & Bretherton, 75 2018; Roh & Song, 2020). Relatively little work has been done to investigate GWPs with 76 ML technqiues. Matsuoka et al. (2020) demonstrated that a convolutional neural net-77 work can estimate the GW structure over Hokkaido, Japan when trained on high-resolution 78 reanalysis data and Chantry et al. (2020) used an artificial neural network (ANN) to em-79 ulate a non-orographic GWP in numerical weather forecasting. 80

We perform a novel investigation into the efficacy of ML as a GWP in a GCM. We 81 demonstrate that the drag due to breaking GWs and resultant circulation can be faith-82 fully generated using an ANN that is trained using data from a global atmospheric model. 83 The ML model, which we call WaveNet, differs from previous work in that it is trained 84 using output from a GCM, provides global coverage, is stable for decadal integrations 85 when coupled to the GCM, and accurately reproduces the large-scale atmospheric circulation. The potential value of a data-driven GWP lies in its computational efficiency after training, its ability to be trained and evaluated using an arbitrary amount of input data, which may include observations, reanalysis, and targeted integrations, and its 89 potential to be appropriated into models containing GWPs thought to be less accurate. 90

91 2 Data

We train the ANN to emulate the M. Alexander and Dunkerton (1999) GWP as 92 incorporated into an atmospheric model of intermediate complexity, the Model of an Ide-93 alized Moist Atmosphere (MiMA) (Jucker & Gerber, 2017; DallaSanta et al., 2019). MiMA 94 captures key dynamical features of the stratosphere-troposphere system that depend crit-95 ically on GWs at a resolution comparable to state-of-the-art stratosphere resolving GCMs. For additional details refer to Jucker and Gerber (2017) and DallaSanta et al. (2019). 97 MiMA is integrated with T42 spectral resolution (triangular truncation at wavenumber 42, roughly equivalent to a 2.8-degree grid) in the horizontal and 40 vertical levels, with 99 a model lid at 0.18 hPa and 23 levels above 100 hPa. 100

The implementation of the M. Alexander and Dunkerton (1999) GWP, hereafter 101 referred to as the AD99 scheme, is based on its formulation within the GFDL Flexible 102 Modeling System. The AD99 scheme aims to capture the effect of non-orographic grav-103 ity wave drag. It is the same scheme employed by GFDL Atmospheric Model 3 (Donner 104 et al., 2011), except modified by Cohen et al. (2013) to ensure that all momentum that 105 reaches 0.85 hPa is uniformly distributed to layers above the stratopause. The scheme 106 assumes a Gaussian spectrum of GWs, discretized as a function of phase speed and launched 107 from the upper troposphere (315 hPa). 108

A broad spectrum of phase speeds is chosen, with a half width of 35 m/s, and cen-109 tered around the speed of the zonal wind at the launch level. The total amplitude of the 110 momentum stress is 0.0043 Pa. The broad spectrum ensures that there is a rich source 111 of GWs at MiMA's lower boundary. The momentum associated with each wave is de-112 posited at its linear breaking level. The intermittency of observed GWs is taken into ac-113 count via a scaling parameter: the breaking level is based on the behavior of a large wave, 114 indicative of the median amplitude of the distribution, but the momentum flux is rescaled 115 to provide the momentum deposition associated with an average wave. This better cap-116 tures the true breaking level of GWs, but smooths out the momentum deposition in time. 117

The chief idealization of the scheme is in our choice of source spectrum. We assume a uniform spectrum that varies only with respect to the zonal winds at the source level. This crudely accounts for filtering of the wave spectrum by the troposphere and was critical for the simulation of the QBO.

We utilized five years of six-hourly output from one integration of MiMA, yielding 11,796,480 training samples per year. The second year of output is used for training, while all others are reserved for testing. Not all runs utilize the full year of training data, and discrepancies are specified per experiment. All training data are standardized by removing the mean and scaling to unit variance, calculated for each variable across each pressure level. Test data was similarly standardized using the mean and variance calculated from training data. Output variables were inverse transformed before presen-tation.

¹³⁰ 3 Neural Network Architecture

An artificial neural network (ANN) is a computing system of interconnected layers of computational nodes. For a detailed review of ANNs, we recommend Brenowitz and Bretherton (2018). We trained two ANNs to generate zonal and meridional drag separately. The ANN architecture is described in Figure S1.

The input layer of both ANNs accepts a single vertical column of resolved flow vari-135 ables from MiMA (Table S1). The output layer produces a single vertical column of 33 136 gravity wave drag (GWD) values, corresponding to the upper 33 model levels (approx-137 imately 0.18hPa to 436hPa). This includes the upper three sponge layers and three lay-138 ers below AD99's average launch level. During online simulations with the ANN, no drag 139 is specified below level 33, i.e. zeros are appended to WaveNet's output to extend to the 140 full length of the vertical column. The result of each node in the output layer does not 141 pass through an activation function. For all other nodes, we use the Rectified Linear Unit 142 (ReLU). In total, this ANN architecture contains 3,848,481 trainable parameters when 143 using the full set of resolved flow variables and shifts slightly, with a lower limit of 3,806,753, 144 when training with a subset of resolved flow variables. 145

The loss function - in our case, the logcosh error - is computed for a minibatch of 1,024 training samples that are drawn from a pseudo-shuffled training dataset. The logcosh error is defined as

$$L(y, y^p) = \sum_{i=1}^n log(cosh(y_i^p - y_i))$$

where n is the size of the dataset and y_i and y_i^p are the i^{th} truth and prediction, respec-149 tively. The logcosh error is found to consistently outperform mean-squared and mean-150 absolute loss functions. Parameter updates are performed according to Adam optimiza-151 tion (Kingma & Ba, 2014). We started each training session with a learning rate of 10^{-3} 152 and reduced it when improvement plateaued for more than 5 epochs, with an epoch de-153 fined as 1,500 batches. We stopped training when performance plateaued for more than 154 10 epochs, which occurred at 200 epochs on average. We did not perform any regular-155 ization. All weights are initialized using Xavier initialization (Glorot & Bengio, 2010). 156

¹⁵⁷ 4 Offline Performance

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4.1 Large-Scale Circulation

We start by training WaveNet on one year of MiMA output and testing it offline on the three years proceeding and one year preceding the training period. In order to assess how well WaveNet captures GWD associated with large-scale circulation, we an-





alyze the vertical profile of drag tendencies at 5°S - 5°N and 60N (Figure 1). WaveNet
is trained on one year of global data (year 2), containing the westward phase of the QBO
and a full seasonal cycle of the polar vortex. The ANN captures the changes in GW driving associated with the eastward phases preceding and proceeding the training period.
The result suggests that WaveNet can transfer learning from regions (horizontally or vertically) containing eastward wind samples to a region where it has not experienced similar samples during the training period.

While comparison between Figure 1a and Figure 1c shows that WaveNet can cap-169 ture the gross features of the "out-of-sample" periods, differences between AD99 and WaveNet 170 are larger at these times, as seen in the middle panel. Notably, the errors decrease around 171 month 48, when the winds are more similar in structure to the training period. This sug-172 173 gests more varied training data or regularization techniques may improve WaveNet's performance. Movies S1-S4 show strong similarities on a global scale between the horizon-174 tal GWD generated by WaveNet and AD99 at 10 hPa and 100 hPa for a six month time 175 series of test data. These results are reassuring with respect to WaveNet's potential to 176 globally generalize from regional observations. 177

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4.2 Interpretability of the ANN

To further evaluate the quality of predictions, we calculate the R^2 coefficient of determination for a one year time series of test data at each spatial location and average for each vertical level. R^2 is defined as one minus the proportion of the sum of squares

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Figure 2. R^2 values are computed for one year of test data at each spatial location and averaged for each model pressure level. Presented are the R^2 values for the feature experiments (a and b), where ten subsets of the full input variable set are provided during training, and data availability experiments (c and d), where the size of the training set is restricted to the number of days specified in the legend.

of residuals to the total sum of squares. We also train WaveNet using ten distinct sub-182 sets of the full resolved flow variable set to determine which training features are most 183 critical (Figure 2ab). When trained with the full feature set (light blue, circle inscribed 184 lines), the average pressure weighted R^2 value above the source level is .91 for zonal and 185 .88 for meridional GWD predictions. Below this level, performance significantly degrades 186 as AD99 overwhelmingly outputs trivial, nonphysical GWD. The zonal (meridional) wind 187 component is the only flow variable necessary to retain 94.4% (96.1%) of the ANN's per-188 formance for zonal (meridional) GWD predictions. 189

To further investigate the role of horizontal wind features, we calculate Shapley Ad-190 ditive Explanations (SHAP) (Lundberg & Lee, 2017a). The SHAP value for a feature 191 is the weighted sum of the conditional expectation of the marginal contribution of in-192 cluding that feature in the prediction. The SHAP values for this study are calculated 193 using Deep SHAP, an approximation technique that combines DeepLIFT with Shapley 194 values from collinear cooperative game theory (Shrikumar et al., 2017; Lundberg & Lee, 195 2017b). Figure S2 shows that on average the horizontal wind components on levels di-196 rectly above and below the level of prediction have the largest contribution to the model's 197

prediction. This is consistent with our physical understanding of GWs, where dissipation is linked to critical levels (i.e., where the phase speed of a wave is equal to the speed of the background flow). This spatially local dependence suggests that our approach may
generalize well to observational datasets that contain measurements at a small range of pressure levels, e.g., observations from superpressure balloons (Podglajen et al., 2016;
Lindgren et al., 2020).

4.3 Sensitivity to Amount of Training Data

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To understand how performance degrades as less training data is made available to the ANN, we incrementally decrease the number of training samples from one year 206 to one day (Figure 2cd). To account for the effects of seasonality, we sample uniformly 207 in space and time from one year of training data to generate a subset with coverage of 208 the entire seasonal cycle. We find that a quarter of a year of data (equivalent to three 200 months or 2.9 million samples) is sufficient to retain 98% of WaveNet's performance com-210 pared to training with one year of data. This suggests the promise of a data-driven GWP 211 to be trained and validated on observational datasets of similar resolution and size, as 212 well as to generalize to simulations that more realistically model the physics of GWs. 213

²¹⁴ 5 Coupling WaveNet with MiMA

Successful offline emulation of key atmospheric structures does not necessarily en-215 gender good online performance. It has been shown that small offline errors can trigger 216 instabilities or accumulate to generate large errors (Brenowitz & Bretherton, 2018). Here, 217 we study the online stability and performance of the emulator by replacing AD99 with 218 WaveNet in MiMA. We couple the ANN, written in Python, with MiMA, written in For-219 tran, by using an interoperability package, forpy. Different approaches can be taken to 220 couple ML algorithms with Fortran (Chantry et al., 2020; Ott et al., 2020). The main 221 advantage of forpy is that it supports complex network structures and requires nominal 222 effort to recouple with alternate ML schemes. The primary disadvantage of this inter-223 face is that it is slow compared with alternate approaches. When coupled, WaveNet slows 224 the entire GCM by roughly 7.5x, a result of the forpy interface and WaveNet's size. The 225 runtime may be further optimized by switching to an alternate coupling interface, per-226 forming quantization and pruning, reducing the number of trainable weights, and mi-227 grating to a GPU compatible GCM. Optimizing and analyzing WaveNet's run-time is 228 a subject of on-going study and beyond the scope of this work. For all subsequent on-229 line analysis, we use the versions of WaveNet trained with one year of data that accept 230 as input (u,T; zonal ANN) and (v,T; meridional ANN). 231

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Figure 3. Pressure-Time profiles of the zonal mean zonal wind, averaged from between 5° S and 5° N and smoothed with a 15-day low pass filter show the behavior of the QBO in 30 year integrations of (a) the control version of MiMA with the AD99 parameterization, (b) the model coupled with WaveNet, (c) a 4xCO2 integration with the AD99 parameterization, and (d) a 4xCO2 integration coupled with WaveNet. Vertical dashed lines separate 5 year segments. The eastward (red) and westward (blue) bands correspond to winds associated with breaking GWs in opposite phases of the QBO. The QBO period and amplitudes are calculated using the transition time (TT) method. The dashed-horizontal line in each panel delineates the model level (≈ 10 hPa) where the TT method is used.

6 Online Performance

To demonstrate the ability of WaveNet to act as a faithful emulator online, we com-233 plete a 30-year integration of MiMA coupled to WaveNet using two configurations. Fig-234 ure 3 shows pressure-time profiles of 15-day averaged zonal mean zonal winds between 235 5°S and 5°N for the two configurations for AD99 (a,c) and WaveNet (b,d). Following 236 the transition time (TT) method described in Richter, Anstey, et al. (2020), we calcu-237 late the period of each QBO cycle as the difference in time between every other phase 238 change for the 5°S to 5°N averaged zonal mean zonal wind time series at roughly 10 hPa. 239 The westerly (easterly) amplitude is taken as the maximum (minimum) value of the time 240 series for each QBO cycle. The numbers in the lower left corner of each panel show these 241 statistics calculated for years 1 through 30 with the spin-up time omitted. From the same 242 experiments, we plot the average zonal winds and temperature as a function of pressure 243 and latitude in Figure 4. 244

6.1 Baseline Emulation

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The first experiment utilizes the same model configuration as was used to gener-246 ate training data and serves to evaluate WaveNet's ability to emulate AD99 while on-247 line. For this scenario, WaveNet produces a QBO with an average period of 30.27 ± 2.82 248 months, slightly longer than the 28.18 ± 2.51 month period generated by AD99. This 249 difference can easily be observed in Figure S3 which shows that the error magnitude os-250 cillates with out-of-phase samples. WaveNet produces remarkable consistency in the over-251 all height and fine-scale features of the QBO. The asymmetry between easterly and west-252 erly amplitudes, which is well appreciated in models and observations (DallaSanta et al., 253 2021), is fully captured by WaveNet. The amplitude fidelity is limited by the training 254 period. The simulated westerlies are too strong compared to those generated by AD99, 255 as the ANN was trained over an easterly dominated year; however the difference between easterly amplitudes is not statistically significant. This suggests that training an ANN 257 on limited observations (less than one QBO cycle) may provide spectral insight even if 258 the entire amplitude cycle is not well-sampled. WaveNet produces a climatology simi-259 lar to AD99 (Figure 4). WaveNet generates a stronger polar vortex (Figure S4) and cooler 260 temperatures (Figure 4j) in the upper atmosphere in both poles. The general agreement 261 between WaveNet and AD99 observed in these results is a strong indicator that WaveNet 262 can act as a faithful emulator of AD99. 263

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6.2 Forcing Emulation

To be useful, a data-driven GWP must accurately emulate GWD across a range of model configurations and scenarios not fully captured in training data. The second experiment presented here serves as a first step towards understanding WaveNet's sensitivity to model configuration. Here, we completed a coupled run using four times preindustrial concentrations of CO2 (1200ppm) or roughly triple that of the baseline run (390ppm), which was optimized for early 21st century scenarios. Figures 3c and 3d show that when using either AD99 or WaveNet the average period and amplitude of the QBO decrease and the variance increases. The amplitude decrease is common among stateof-the-art models (Richter, Butchart, et al., 2020) and is attributed to increased tropical upwelling, which is separate from GWD. However, we observe that the QBO generated by WaveNet has a larger response to forcing and enhanced variance.

Models differ regarding the period projection; and a mechanism is not yet clear, 276 as the intermodel correlation between period decrease and increased gravity wave flux 277 vanishes when only fixed-source GWPs are considered (Richter, Butchart, et al., 2020). 278 Thus, it is significant that AD99 and WaveNet project similar changes to QBO period, 279 highlighting the role of changes in the background state. Our idealized model results point 280 to further investigation with more complex models, e.g. within the GFDL Flexible Mod-281 eling System. Figure 4 and Figure S4 show that WaveNet and AD99 have a very sim-282 ilar climatological response to external forcing (e.g. both produce stronger polar jets and 283 similar tropical changes). Although the regions that are statistically distinguishable vary, 284 likely due to changes in regional variability, the fraction of total distinguishable points 285 remains roughly the same for the 4xCO2 (36% u, 31% temp) and baseline scenarios (39% 286 u, 28% temp). 287

²⁸⁸ 7 Discussion and Conclusion

We have demonstrated that an ANN can skillfully learn the salient features of GW 289 momentum transport directly from resolved flow variables. We have produced an em-290 ulator that can stably run when coupled with a simplified global atmospheric model for 291 multidecadal time-periods and reproduce the large-scale circulation. We have shown that 292 the most important input features for WaveNet's predictions are the horizontal wind com-293 ponents local to the vertical level of prediction, and we have demonstrated that WaveNet 294 can generalize using limited training data, online and offline. Finally, WaveNet produces 295 a climatological response to CO2 forcing similar to that generated by AD99. The suc-296 cess of these experiments implies that an approach like WaveNet may open a new av-297 enue by which the advantages of high-resolution GW simulations (Remmler et al., 2015) or observational datasets (Lindgren et al., 2020) can be incorporated into current GCMs. 299

There are, however, a number of challenges that may emerge before the advantages of an approach like WaveNet can be fully realized in a GCM. First, ANNs do not inherently conserve energy or momentum. Second, the lack of interpretability of ANNs may serve as a substantial barrier to their widespread adoption. Additional effort is necessary to consider how WaveNet's behavior may relate to the GW dispersion relations. Third, WaveNet in its current setup is too slow. In order to make coupling WaveNet with a GCM computationally feasible, a cost-performance analysis is planned to reduce WaveNet's



Figure 4. Pressure-Latitude profiles of average temperature (a,b) and zonal winds (g,h) in the baseline (a,g) and 4xCO2 (b,h) simulations for AD99. Panels d, e, j, and k present the climato-logical difference between AD99 and WaveNet for average temperature and zonal winds for the baseline and 4xCO2 simulations. Regions that are statistically distinguishable (p<0.05) via the Student's t-test are dotted. The climate change signal for average temperature and zonal winds for WaveNet and AD99 are presented in the rightmost column.

³⁰⁷ complexity, optimize coupling, and utilize GPU hardware. A next test is to examine how

WaveNet generalizes when run using various model configurations and trained on regional datasets and orographic and nonorographic GWPs.

Nevertheless, our results suggest that machine learning may represent a powerful alternative to existing GWPs. The approach presented here constitutes a first step toward obtaining such GWPs for global climate prediction.

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321 Data Availability

The ANN is built using Keras, a deep learning framework that wraps Tensorflow. 322 All training source code is available at https://doi.org/10.5281/zenodo.4428931 (Espinosa, 323 2021). Training took on the order of 12 hours on a graphical processing unit and var-324 ied according to data size and trainable parameters. The implementation of SHAP val-325 ues is available at https://github.com/slundberg/shap and is not maintained or owned 326 by this project group (Lundberg & Lee, 2017a). MiMA is documented by Jucker and Ger-327 ber (2017) and Garfinkel et al. (2020), maintained at https://github.com/mjucker/ 328 MiMA and available at https://zenodo.org/record/3984605#.YVYXtzHMKHs. The model 329 code, forpy coupling code, trained ANNs, run parameters, and modified configuration 330 for MiMA are available at https://zenodo.org/record/5533166. The coupling library, 331 forpy, developed and maintained by Elias Rabel is well documented and available at https:// 332 github.com/ylikx/forpy (Rabel et al., 2018). 333

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Figure 1.

Zonal Mean Zonal Gravity Wave Drag (5°S - 5°N)



Zonal Mean Zonal Gravity Wave Drag (60°N)







Figure 2.



Figure 3.



Figure 4.

