A New Four-Component L*-dependent Model for Radial Diffusion based on Solar Wind and Magnetospheric Drivers of ULF Waves

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Abstract

Waves which couple to energetic electrons are particularly important in space weather, as they drive rapid changes in the topology and intensity of Earth's outer radiation belt during geomagnetic storms. This includes Ultra Low Frequency (ULF) waves that interact with electrons via radial diffusion which can lead to electron dropouts and rapid acceleration and inward transport of electrons during. In radiation belt simulations, the strength of this interaction is specified by ULF wave radial diffusion coefficients. In this paper we detail the development of new models of electric and magnetic radial diffusion coefficients derived from in-situ observations of the azimuthal electric field and compressional magnetic field. The new models use L^* as it accounts for adiabatic changes due to the dynamic magnetic field coupled with an optimized set of four components of solar wind and geomagnetic activity, B_z, V, P_{dyn} and $Sym\text{-}H$, as independent variables (inputs). These independent variables are known drivers of ULF waves and offer the ability to calculate diffusion coefficients at a higher cadence then existing models based on Kp. We investigate the performance of the new models by characterizing the model residuals as a function of each independent variable and by comparing to existing radial diffusion models during a

38   quiet geomagnetic period and through a geomagnetic storm. We find that the models developed here

39   perform well under varying levels of activity and have a larger slope or steeper gradient as a function of

40   L^* as compared to existing models (higher radial diffusion at higher L^* values).

Plain Language Summary

42   The outer radiation belt is a region of space comprising highly energetic electrons. During periods of

43   extreme space weather, the number and energy of these electrons can rapidly vary. During these

44   periods as the electron energies and numbers become enhanced, they can pose a threat to satellite and

45   space infrastructure. While we have an excellent understanding of the physical processes which drive

46   radiation belt electron dynamics, we still have a limited ability to model and forecast radiation belt

47   dynamics; this is a result of the complexity of Earth's radiation belt system. One of the key processes

48   controlling radiation belt dynamics is Ultra Low Frequency (ULF) wave radial diffusion. In this work we

49   detail the development a new model quantifying the strength of Ultra Low Frequency (ULF) wave radial

50   diffusion in the outer radiation belt utilizing space base observations of the electric and magnetic fields

51   in Earth's magnetosphere. Accurately quantifying ULF wave radial diffusion is fundamental to

52   understanding radiation belt dynamics and any improvement or refinements in radial diffusion models

53   can help to provide a better understanding of the complex radiation belt system and importantly

54   improve hindcasts, nowcasts, and forecasts.

1 Introduction

The Earth's outer radiation belt is a toroidal region between ~2-8 R_E comprising energetic electrons from hundreds of keV to several MeV (Mauk et al., 2013). Periods of elevated solar activity, such as coronal mass ejections, corotating interaction regions, dynamic solar wind, and interplanetary shocks can drive increased geomagnetic activity leading to rapid changes in the flux of energetic electrons and enhancements of the terrestrial ring current (e.g., Kanekal & Miyoshi, 2021). These periods of enhanced geoeffective solar wind are referred to as geomagnetic storms. During these storms the enhanced fluxes of the radiation belt can be dangerous for human and robotic space activity as well as causing damage to sensitive spacecraft systems (e.g., Baker 2001; Cassak et al., 2017).

Though the outer radiation belt was discovered over half a century ago (Van Allen & Frank, 1959), our understanding of, and ability to model and forecast its dynamics remains somewhat limited. This is not a result of a lack of understanding of the processes which drive radiation belt dynamics but instead is due to the complexity and variability of the overall system, from the sources and sinks of electrons and wave-particle interactions coupling to these electrons, to the cross-coupling with other magnetospheric regimes such as the magnetopause (e.g., Borovsky & Valdivia, 2018; Halford et al., 2022; J. Rae et al., 2022). During storms, the dynamics of the radiation belt are controlled by a variety of physical processes leading to loss, transport, and acceleration of electrons. For instance, magnetopause shadowing (Staples et al., 2022; West et al. 1972) coupled with outward radial diffusion driven by Ultra Low Frequency (ULF) waves (e.g., Turner et al., 2012) can drive rapid losses of electrons. At the same time wave-particle interactions driven by Very Low Frequency (VLF) Chorus and Hiss waves (e.g., Breneman et al., 2015; Halford et al., 2022; O'Brien et al., 2004), electromagnetic ion cyclotron waves (EMIC) (e.g., Bingley et al., 2019; Bruno et al., 2022), ULF waves (e.g., Brito et al., 2015; Rae et al. 2018), and kinetic Alfven (e.g., Chaston et al., 2018) waves can enhance electron precipitation across a wide range of energies leading to a loss of radiation belt electrons. Further, enhanced convection and substorm injections can replenish lower energy electrons providing pathway for the excitation of whistler mode chorus which can rapidly accelerate electrons to relativistic (several MeV) energies (Horne 2003; Horne and Thorne 1998; Horne et al. 2005; Thorne et al., 2013) creating peaks in electron phase space density (Reeves et al., 2013). ULF (Ozeke et al. 2014) waves can further rapidly accelerate and transport these lower energy seed electrons to MeV energies via ULF wave radial diffusion.

The evolution of the radiation belt is controlled by the sum of the effects of the physical processed described above, and whose strengths varies throughout any given storm leading to a variety of responses. For example, while loss processes typically dominate during the early part of geomagnetic storms (Murphy et al. 2018), the relative strength of these processes varies through the course of a storm and for storm to storm. This variation can lead to striking differences in the topology of the outer radiation belt such as the formation of multiple outer radiation belts (Baker et al. 2013). Following this initial period of loss, the outer radiation belt typically experiences a short period of rapid acceleration (Murphy et al. 2018). However, the dominant process controlling this acceleration can also vary from storm to storm (Ma et al., 2018) and though this period of acceleration is typical of all storms, the amount of acceleration varies (Murphy et al. 2020). This delicate balance between loss, acceleration and transport processes is often referred to as a competition. However, it's more a symphony than a

95   competition; an orchestra of physical processes of varying magnitudes working in concert to shape the

96   topology of the radiation belt through the course of a geomagnetic storm.

97   Fully understanding the dynamics of the outer radiation belt requires at least three key steps. First we

98   need to be able to quantify the strength of physical processes controlling these dynamics. Second, we

99   need to assess how the varying strength of the processes act together to impact the overall topology of

100   the outer radiation belt. Finally, we need understand the pre-existing state of the belts (e.g. initial

101   conditions), and the availability or lack thereof of various source populations (e.g., boundary conditions)

102   through the course of a storm.

103   ULF wave radial diffusion is a key physical processes controlling the dynamics of the outer radiation belt

104   (Schulz & Lanzerotti, 1974). Depending on the gradient of electron phase space density in the outer

105   radiation belt ULF wave radial diffusion can drive either rapid loss or rapid acceleration of radiation belt

106   electrons (Figure 16 of Li & Hudson, 2019; Figure 3 of Turner et al., 2012) across a wide range of

107   energies. In this paper we detail the development of a new model for electric and magnetic ULF wave

108   radial diffusion coefficients, D_{LL}^E and D_{LL}^B, driven by both solar wind input and geomagnetic activity and

109   addressing the first of the three steps described above. This is a more detailed approach which allows

110   the model to account for variability in radial diffusion as well as allowing the model to have a higher

111   cadence than existing models based on a single low resolution independent variable Kp. The new model

112   is derived from in-situ observations of the azimuthal electric field and compressional magnetic field

113   which are used to create a database of satellite-derived D_{LL}^E and D_{LL}^Bs. Using this database, we further

114   characterize the performance of the models and identify, quantify, and remove biases in the model to

115   provide an overall improved model of both D_{LL}^E and D_{LL}^B. Accurately quantifying ULF wave radial

116   diffusion is fundamental to understanding the spatio-temporal dynamics of the radiation belt. Thus, any

117   improvement or refinements in the quantification of the rates of ULF radial diffusion coefficients can

118   increase the fidelity of radiation belt simulations. This in turn can provide better hindcasts, nowcasts,

119   and forecasts of the outer radiation belt, and thus deliver a better understanding of the complex system

120   of wave-particle interaction processes described above and which act in concert to produce the

121   observed radiation belt response.

122   In the subsequent sections we detail the data and methodology used to calculate satellite-derived ULF

123   wave radial diffusion coefficients. This is followed by a description of the development of the D_{LL}^E and

124   D_{LL}^B models, including a parametric study to identify the best set of solar wind and geomagnetic

125   variables to use, and an investigation of the performance and bias of the new models as a function of

126   independent variable. The new D_{LL}^E and D_{LL}^B models are then compared to existing models of ULF wave

127   radial diffusion during an interval of quiet geomagnetic activity as well as during a geomagnetic storm.

128   These results are then summarized and we conclude with future work and potential directions for future

129   research.

130   **2   Data and Methodology**

131   In this work we utilize in-situ observations of ULF wave fluctuations to develop an analytic model of ULF

132   wave electric and magnetic radial diffusion coefficients (D_{LL}^E and D_{LL}^B) which can be used in radiation belt

133   simulations. To achieve this, observations of the inner-magnetosphere magnetic and electric field from

134   the Time History of Events and Macroscale Interactions During Substorms (THEMIS) probes

135   (Angelopoulos, 2008; Sibeck & Angelopoulos, 2008), the two Van Allen Probes (Mauk et al., 2013), and

136   magnetic field data from the Operational Environment 15 (NOAA GOES-15) satellite (Singer et al., 1996)

137   from a similar time period are used (2012-2020). From these data, we develop a database of ULF wave

138   power spectral density (PSD), calculate satellite-derived D_{LL}^E and D_{LL}^B from the PSD database, and

139   subsequently derive an analytic model of both D_{LL}s. Supporting Information Table S1 lists the satellites,

140   time period, instruments, and observables used to calculate the electric and magnetic ULF wave PSD.

141   These PSD are then used to estimate the magnetic and electric D_{LL}s. In addition to the in-situ

142   magnetospheric observations, we also use the OMNI dataset (King & Papitashvili, 2005), and the

143   SpacePy (Niehof et al., 2022) and International Radiation Belt Environment Modeling (IRBEM) libraries

144   (Boscher et al., 2022) to parameterize the derived PSD and D_{LL}s as function of prevailing solar wind,

145   geomagnetic conditions, and third adiabatic invariant L^*. In this study we use the TS05 magnetic field

146   model (Tsyganenko & Sitnov, 2005) to derive L^* using the (IRBEM) library (Boscher et al., 2022) assuming

147   a 90° local pitch angle. The OMNI data set and L^* are used as independent variables (or inputs) to train

148   our radial diffusion models (Section 3). Note, we only use GOES West as it is closer to the magnetic

149   equator then GOES East and therefore provides a better estimate of equatorial ULF wave PSD. This

150   requirement, along with ensuring that the missions overlap in time, means that only GOES-15 is used in

151   this study. Further, we use THEMIS A, D, and E as during the period of interest the other two probes are

152   orbiting the moon. Finally, we use L^* rather then L or radial distance as it more accurately characterizes

153   the topological state of the outer radiation belt as it accounts for adiabatic changes due to dynamic

154   changes in Earth's magnetic field. In the following subsections we describe the methodology for

155   calculating ULF wave PSD as well as the methodology to estimate radial diffusion coefficients from the

156   derived PSDs.

2.1 ULF Power Spectral Density

158   Estimating ULF wave radial diffusion coefficients requires the compressional magnetic field $\boldsymbol{B}_{\parallel}$ and

159   azimuthal electric field $\boldsymbol{E}_{\varphi}$ power spectral density (PSD) (e.g., Fei et al., 2006; Ozeke 2014). To calculate

160    $\boldsymbol{B}_{\parallel}$ and $\boldsymbol{E}_{\varphi}$ we follow the same general framework utilized within the community (e.g., Ali et al., 2015;

161   Ozeke et al. 2014). For each satellite the magnetic and electric fields are rotated into a field aligned

162   coordinate system using a twenty-minute average of the background field to obtain the compressional

163   magnetic field $\boldsymbol{B}_{\parallel}$ and azimuthal electric field $\boldsymbol{E}_{\varphi}$. From $\boldsymbol{B}_{\parallel}$ and $\boldsymbol{E}_{\varphi}$ the PSD can be calculated using

164   several methods such as the multi-taper (Ali et al., 2015; Bentley et al., 2018), wavelet (Dimitrakoudis et

165   al., 2015; Sandhu et al., 2021), or the Fourier transform (Murphy et al. 2011; Rae et al. 2012). In general,

166   each method produces similar estimates of the PSD. Here we use the Fourier transform method outlined

167   in Rae et al. (2012) which has been used in several studies for quantifying ULF wave PSD (Murphy et al.

168   2011; Murphy et al. 2018) as well as subsequently estimating radial diffusion coefficients (e.g., Ma et al.,

169   2018; Mann et al., 2016; Ozeke et al. 2017; Ozeke et al. 2014). Using this method, the $\boldsymbol{B}_{\parallel}$ and $\boldsymbol{E}_{\varphi}$ PSD is

170   calculated for each satellite from a twenty-minute time window stepped by five minutes. Each PSD is

171   then tagged with the prevailing solar wind and geomagnetic conditions from the OMNI database and

172   the satellites position in L^* corresponding to the middle of the 20-minute window (spectra with no

173   corresponding OMNI or L^* data are dropped from the database).

174   There are several caveats to note in the calculation of the field aligned coordinates and of the electric
175   and magnetic field PSD. First, the datasets in Table S1 all have different cadences, and so, prior to
176   calculating the PSD, $B_\parallel$ and E_φ are downsampled to 12s so that all time-series have the same cadence.
177   Second, at low L-shells THEMIS and Van Allen Probes rapidly move through L leading to large variations
178   in the background magnetic field. This introduces artificial power into the magnetic field ULF wave PSDs.
179   To circumvent this, for the Van Allen Probes below L = 4 we remove a third-degree polynomial from $B_\parallel$;
180   this removes the background magnetic field while aiming to retain the ULF wave fluctuations. Further,
181   we limit Van Allen Probe data to L >3 R_E, whilst for THEMIS data we limit observations to L > 5. Different
182   limits are chosen due to the different rates at which these different satellites cross L along their orbit.
183   Third, both THEMIS and the Van Allen Probes measure with high-fidelity long-wire antennas a two-
184   component electric field in the spin plane; in this study we utilize the Level-2 THEMIS EFI data and Level-
185   3 Van Allen Probes EFW data, both which use the $E \cdot B = 0$ approximation to estimate the third
186   component of the electric field. THEMIS data is further calibrated using SPEDAS (Angelopoulos et al.,
187   2019) while Van Allen Probes Level-3 data has undergone extensive processing by the EFW team
188   (Breneman et al., 2022). Finally, regardless of calibration and data processing it is still possible for poor
189   quality electric and magnetic field data to exist leading to anomalous PSDs. Thus, both the $B_\parallel$ and E_φ
190   PSD spectra are further scrubbed by identifying and removing outliers using the following analysis:

191   1. Calculate the summed PSD for each of $B_\parallel$ and E_φ spectra between 0.83-15 mHz.
192   2. Bin the summed PSD datasets by Kp and L-shell.
193   3. Calculate the interquartile range (IQR) of each bin (upper quartile-lower quartile, Q_U-Q_L)
194   4. Identify outlying spectra as any spectra whose summed PSD is less than Q_L-1.5*IQR or greater
195   than Q_U+1.5*IQR and are removed from the PSD data set.

196   This method of scrubbing data and removing outliers is often used in statistical analysis and data
197   sciences. In our study, this method does an excellent job removing anomalously high power associated
198   with erroneous or unphysical data. For example, prior to removing outliers the mean spectrum is larger
199   than the upper quartile spectra. Once the outliers are removed, the mean spectrum closely follows the
200   upper quartile spectrum; though this still represents a skewed distribution, the similarity between the
201   mean and upper quartile is in agreement with previous statistical studies of ULF wave PSD (e.g., Bentley
202   et al., 2018; Murphy et al. 2011).

203　Once processed, scrubbed, and tagged with the OMNI data and L^* position there are over 1.7 million
204　magnetic and 0.46 million electric field PSD which span nearly an entire solar cycle and cover the entire
205　inner magnetosphere through a variety of solar wind and geomagnetic conditions. Figure 1 shows the
206　median $\boldsymbol{B}_{\parallel}$ (top) and $\boldsymbol{E}_{\varphi}$(bottom) PSD at each frequency (y-axis) as function of Kp (x-axis) and L^* (panels
207　1-8). Evident in Figure 1 is that power is concentrated at lower frequencies and increases at all
208　frequencies with Kp, consistent with previous studies (Ali et al., 2015; Brautigam & Albert, 2000; Rae et
209　al. 2012). Panels 9 of Figure 1 (far right) shows how the PSD varies with L^* and Kp at a fixed frequency of
210　2.5 mHz. Consistent with previous studies this final panel demonstrates that ULF wave PSD increases
211　with both L^* and geomagnetic activity as parameterized by Kp. The database of PSD spectra described
212　and shown in Figure 1 is used to estimate D_{LL}^E and D_{LL}^B as described in the next subsection.
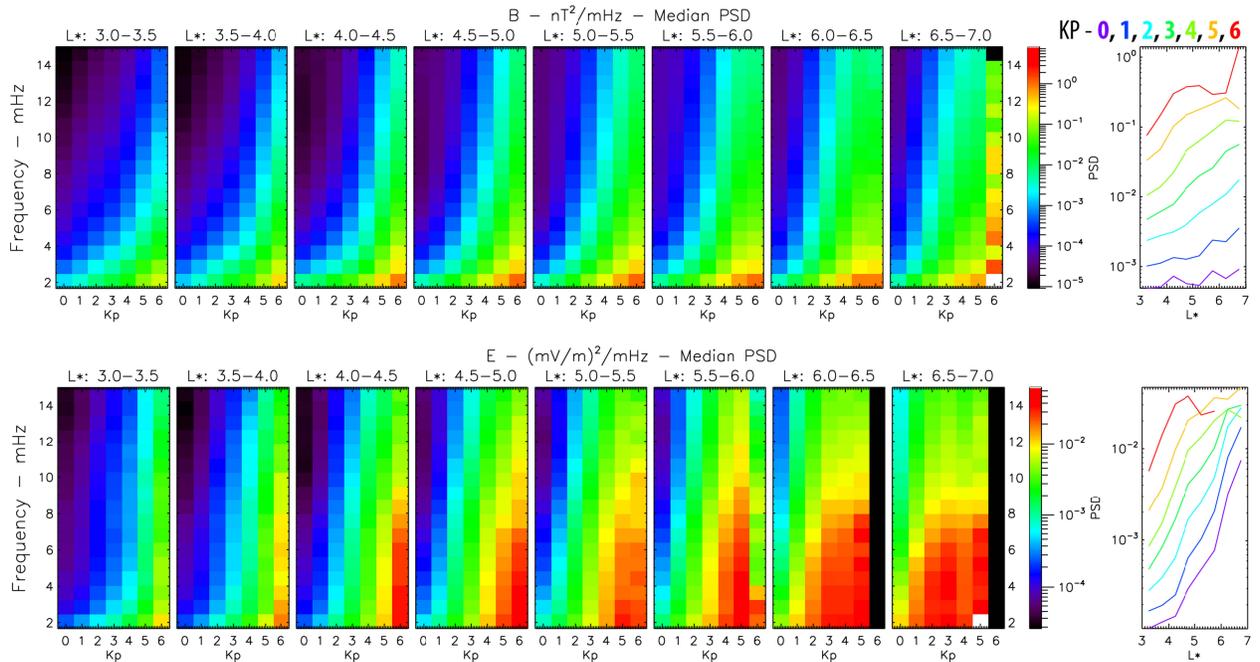
213

214　Figure 1: Statistical variation of the $\boldsymbol{B}_{\parallel}$ (top) and $\boldsymbol{E}_{\varphi}$(bottom) PSD. The spectral plots show the median PSD as a
215　function of frequency (y-axis), Kp (x-axis) and L^* (panels 1-8). The line plots show the variation of PSD at fixed a
216　frequency of 2.5 mHz as a function of L^* and Kp (color) for the entire dataset.

2.2 Radial Diffusion Estimation

218　Radial diffusion coefficients can be calculated in several ways (e.g., Fei et al., 2006; Schulz & Lanzerotti,
219　1974). In this work, since we are utilizing $\boldsymbol{B}_{\parallel}$ and $\boldsymbol{E}_{\varphi}$ we use the framework outlined by Ozeke et al.
220　(2014) and Mann et al. (2016) which follows the Brizard and Chan (2001) and Fei et al. (2006) formalism.

221　Ozeke et al. (2014) developed expressions for the electric and magnetic radial diffusion coefficients
222　which depend on the azimuthal electric field and compressional magnetic field PSD and which are
223　energy and azimuthal wave number independent (see equations 19 and 22). In their work Ozeke et al.
224　(2014) used in-situ THEMIS and GOES observations to quantify the compressional magnetic field $\boldsymbol{B}_{\parallel}$ PSD
225　and ground-based magnetometer observations to quantify the azimuthal electric field $\boldsymbol{E}_{\varphi}$ PSD. The

226   statistical variation of these PSD as a function of Kp were substituted into equations 19 and 22 to derive
227   analytical Kp dependent function of D_{LL}^B and D_{LL}^E.

228   In a follow on study, Mann et al. (2016) expanded on the Ozeke et al. (2014) framework to derive event-
229   specific D_{LL}^Es from ground-based magnetometers. Mann et al. (2016) averaged the ULF wave PSD over a
230   fixed frequency range and substituted it into equation 22 of Ozeke et al. (2014) to derive time-
231   dependent-event-specific diffusion coefficients. In their study Mann et al. (2016) used these event
232   specific diffusion coefficients to model the formation of the outer and storage radiation belts observed
233   by the Van Allen Probes in September 2012 (Baker et al. 2013). These authors demonstrated that event-
234   specific ULF wave radial diffusion coefficients coupled with dynamic boundary conditions reproduced
235   the double belt structure of the outer radiation belt, highlighting the importance of ULF wave radial
236   diffusion in controlling the dynamic topology of the outer radiation belt. Several follow-on studies have
237   used the same methodology as Mann et al. (2016) to derive event-specific ULF wave radial diffusion
238   coefficients to study the importance of radial diffusion radiation belt dynamics. In general, these studies
239   have demonstrated that radiation belt simulations using event specific radial diffusion coefficients
240   perform better, in that they more accurately reproduce radiation belt electron dynamics, than those
241   that do not (Ma et al., 2018; L. G. Ozeke et al., 2019, 2020).
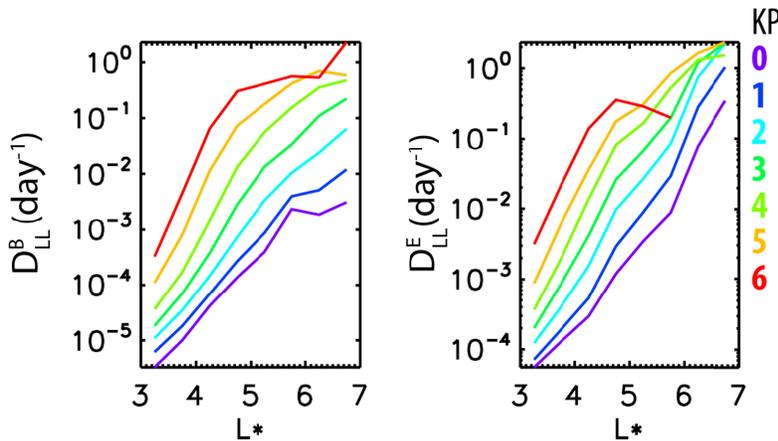

243   Figure 2: Median D_{LL}^B (left) and D_{LL}^E (right) as function of L^* and Kp for the entire dataset.

244   Here, we use the same approach as Mann et al. (2016) to derive in-situ D_{LL}^E and D_{LL}^B from the $\boldsymbol{E}_\varphi$ and $\boldsymbol{B}_\parallel$
245   PSD using equations 19 and 22 from Ozeke et al. (2014). Each spectrum from the PSD database is
246   averaged between 0.83-15.00 mHz. The averaged $\boldsymbol{B}_\parallel$ and $\boldsymbol{E}_\varphi$ PSD are then substituted into equations 19
247   and 22 of Ozeke et al. (2014) providing an energy and azimuthal wave number independent estimate of
248   D_{LL}^B and D_{LL}^E respectively. Figure 2 shows the median D_{LL}^B (left) and D_{LL}^E (right) as a function of L^* and Kp.
249   The D_{LL}s are similar in magnitude to other studies and increase with L^* and increasing geomagnetic
250   activity (e.g., Ozeke et al. 2014). At higher Kp values (e.g., 5 and 6), the magnitude of D_{LL}^B is comparable
251   to D_{LL}^E. This is consistent with recent work that has demonstrated that during the main phase of storms
252   the magnitude of $D_{LL}^B \sim D_{LL}^E$ (Olifer et al., 2019; Sandhu et al., 2021). It is important to note that in this
253   approach $\boldsymbol{E}_\varphi$ and $\boldsymbol{B}_\parallel$ are treated independently whereas in fact they fact they are correlated via
254   Faraday's law. In addition, the electric field includes both the electrostatic as well as the

255 electromagnetic component. Regardless, recent work has demonstrated that the resulting diffusion
256 coefficients are within a factor of approximately two of the electromagnetic diffusion coefficients
257 (Lejosne, 2019). In the next section we describe the development of a radial diffusion model utilizing the
258 database of D_{LL}s described here.

3 Radial Diffusion Model

260 ULF wave radial diffusion is a key component of radiation belt dynamics, driving periods of enhanced
261 electron loss via outward radial transport as well as electron acceleration via inward transport (e.g.,
262 Ozeke et al. 2017). In radiation belt models, the strength of ULF wave radial diffusion is specified by
263 diffusion coefficients D_{LL} (e.g., Brizard & Chan, 2001; Fei et al., 2006). Several researchers have
264 developed models which specify the strength of radial diffusion coefficients as a function of
265 geomagnetic activity from both in-situ and ground-based observations of ULF wave PSD (Ali et al., 2015;
266 Brautigam & Albert, 2000; Ozeke et al. 2014). In this section we build on these studies using a database
267 of satellited-derived ULF wave D_{LL}^{E} and D_{LL}^{B} radial diffusion coefficients in an attempt to develop a more
268 robust characterization of the rates of ULF wave radial diffusion based on known drivers of ULF waves.
269 Here we describe the development of the radial diffusion model including a parametric study to identify
270 a robust set of independent variables as model inputs, a discussion of different model types/algorithms,
271 and training, testing, and performance of a final model. In section 4 we investigate the final model,
272 including its performance under different geomagnetic conditions (e.g., quiet and storm times) and
273 comparing to existing diffusion models.

3.1 Parametric Study

275 Previous studies developing radial diffusion models parameterized their diffusion coefficients based on
276 the planetary index Kp. Kp is a three-hour index ranging from 0 to 9; the indices correspond to
277 exponentially increasing perturbations of Earth's magnetic field as characterized by several ground-
278 based magnetometers from around the world. While Kp is a good measure of geomagnetic activity, its
279 utility in models is limited for three reasons. First, Kp is a measure of the response of the coupled solar
280 wind-magnetosphere-ionosphere system as opposed to a driver of the dynamics of this system. Second,
281 the three-hour cadence is long compared to storm-time radiation belt time-scales (Olifer et al., 2018;
282 Ozeke et al. 2017). Finally, the exponentially increasing index limits the dynamic range of models,
283 requiring models to extrapolate to high values of Kp during very active times. For example, the
284 Brautigam and Albert (2000) and Ozeke et al. (2014) models are limited to using data derived for
285 conditions with Kp≤6 while Liu et al. (2016) and Ali et al. (2016) diffusion models are limited to a
286 maximum Kp value of 5. Above these values the respective models must extrapolate to higher Kp values
287 to estimate the magnitude of radial diffusion coefficients under active conditions. Despite these
288 limitations, there is a key advantage in that the D_{LL}s parameterized by Kp in that they can be easily
289 forecasted when forecasts of Kp are readily available (Glauert et al., 2021; Horne et al. 2021).

290 In this work we use the OMNI dataset to parameterize and develop models of radial diffusion at higher
291 cadence using known drivers of ULF waves. The OMNI data has a higher cadence (1 hour, 5 minute, and
292 1 minute) than the Kp index. This is ideal for radiation belt models as it provides increased temporal
293 dynamics and resolution. In addition, the OMNI dataset contains multiple parameters including the solar
294 wind vector magnetic field, dynamic pressure, the vector solar wind velocity, as well as multiple

295 geomagnetic indices. This allows for the development of models with multiple inputs which can increase

296 model performance; however, one must identify an ideal set of inputs which maximizes model

297 performance, while maintaining model stability (e.g., modelled D_{LL}s do not exhibit high variance with

298 certain combinations of variables) and simplicity (e.g., avoiding the addition of variables with little

299 impact).

300 In our development of new parameterizations of D_{LL}^B and D_{LL}^E we perform a parametric study of L^* a

301 proxy of the third adiabatic invariant, $Sym\text{-}H$, the GSM y and z components of the interplanetary

302 magnetic field (IMF; B_y and B_z), solar wind speed V and x-component V_x GSM, and the solar wind

303 dynamic pressure (P_{dyn}) and density (n) to identify the best combination of independent variables (or

304 inputs) with which to develop models of D_{LL}^B and D_{LL}^E. From this set of independent variables, L^* is the

305 only required variable in our model as it defines the radial diffusion coefficients on a set grid as is

306 required for its implementation in radiation belt simulations. Unlike other models we use L^* as it is more

307 physically meaningful then radial distance or L as it accounts for adiabatic changes due to the dynamic

308 magnetic field. The other independent variables selected for our parametric study correspond to known

309 drivers of ULF wave power in the magnetosphere (Bentley et al., 2018; Kepko et al., 2002; Mathie &

310 Mann, 2001; Murphy et al. 2015; Rae et al. 2019).

311

312 Figure 3: Results of the parametric study. (a) and (b) Correlation and mean square error (MSE) of data and multi-
313 linear regression model for all combinations of independent variables (identified as integers on the x-axis). (c) A
314 zoom in of (a) and (b) highlighting the combination of independent variables resulting in a high correlation and low
315 MSE between the data and multi-linear regression model; the black line is the correlation and blue the MSE, the x-
316 axis shows the various combinations of independent variables.

317 To identify an optimized set of independent variables the parametric study loops through every

318 combination of input variables and fits a multi-linear regression model to the $\log_{10}$ of D_{LL}^B. For each

319 model we determine the model-data correlation and mean square error (MSE). Using the correlation

320 and MSE we identify the best combination of independent variables to subsequently train final models

321 of D_{LL}^B and D_{LL}^E. Figure 3 shows the results of this parametric study; panels a and b show the correlation

322 and MSE for every combination of variables (identified simply as integers on the x-axis). Evident in

323 panels a and b is that the correlation increases and MSE decreases for different combinations of inputs.

10

324 Figure 3c focuses on the combination of variables which maximize the correlation and minimize the MSE

325 of the trained model. Evident in Figure 3c is that combinations of L^*, $Sym\text{-}H$, IMF B_z and P_{dyn} coupled

326 with various combinations of IMF B_y, V, V_x, and n all lead to high correlations and low MSE. The

327 correlation peaks and MSE minimizes when all input variables are used in the parametric study;

328 however, this introduces significant multicollinearity between the input variables (e.g., B_z and B_y, V and

329 V_x) which can decrease model performance as well as adding additional complexity. From the

330 parametric study, L^*, $Sym\text{-}H$, B_z, V, and P_{dyn}, are identified as an optimized set of input parameters to

331 model D_{LL}^B (vertical line Figure 3c); the correlation is high, MSE low, and the correlation between input

332 variables is limited compared to the other combination of inputs while also maintaining a level of

333 simplicity by including only five independent variables. A similar dependence has also been discussed by

334 Dimitrakoudis et al. (2022), albeit for ULF wave power which is directly related strength of radial

335 diffusion. Finally note, that the correlations and MSE for this set of independent variables is on the same

336 order as those when Kp and L^* are considered as independent variables. However, in this paper we

337 focus on developing a model based on known drivers of ULF wave power as opposed to variables and

338 indices which respond to ULF wave power and enhanced geomagnetic activity like Kp. Thus, for the

339 purpose of this study the combination of L^*, $Sym\text{-}H$, IMF B_z, V, and P_{dyn} are used as independent

340 variables train models of D_{LL}^B and D_{LL}^E.

341 3.2 D_{LL} Model

342 There are several methods and algorithms which could be used to generate or train models for the

343 parameterization of the electric and magnetic field D_{LL}s. In this work we investigated two algorithms for

344 training models of D_{LL}^B and D_{LL}^E, a multi-linear regression model (Murphy et al. 2015, 2020), and a neural

345 network model (Bortnik et al., 2018). In general, both the multi-linear regression and neural network

346 models performed similarly using the independent variables identified in Section 3.1; both algorithms

347 produced similar correlations and MSEs when fitted to D_{LL}^B and D_{LL}^E. Given the similar model

348 performance, we use a multi-linear regression model for the final parameterisation we present here due

349 to its simplicity as compared to the implementation, use, and sharing of neural networks.

350 In developing the multi-linear regression models, the D_{LL}^B and D_{LL}^E datasets are first regularized as a

351 function of L^*. The regularization ensures that the distribution of D_{LL}s as a function of L^* is uniform, i.e.,

352 the number of D_{LL} data points for any given L^* is the same. This is important as the spacecraft spend

353 more time at apogee, high L^*, which can bias any model by fitting to the bulk of the data which are

354 preferentially located in one part of the domain. The datasets are then randomly separated into

355 train/test sets using a 70/30 percent split. The models are trained on the train set while the test set is

356 used to verify performance. Before training, the independent variables are normalized between 0 and 1

357 by the maximum and minimum values in the train set; this normalization ensures the dependence on

358 each of the independent variables is assessed on a similar scale and generally increases the stability and

359 performance of the resulting models. Finally, we restrict the model space to $L^* \in [3,7]$; this

360 encompasses the outer radiation belt and in general improves model performance by removing highly

361 variable data at higher L^*. Though this limits the dynamic range of the data used to train the linear

362 regression models, the linear regression models can still be used calculate D_{LL}s outside this range.

363 However, care must be taken when extending the model outside these limits as it is not possible to test

364   the models performance in these regions. This final dataset is then fitted to the $\log_{10}$ of D_{LL}^B and D_{LL}^E

365   following the functional form shown in Equation 1; the D_{LL}s can then be calculated as shown in

366   Equation 2.

367
$$log_{10}(D_{LL}) = c + a_1 L^* + a_2 Sym\text{-}H + a_3 B_z + a_4 V + a_5 P_{dyn} \quad (1)$$

368
$$D_{LL} = 10^{c + a_1 L^* + a_2 SymH + a_3 B_z + a_4 V_t + a_5 P_{dyn}} \quad (2)$$

369   Figure 4 shows the results of the training of the linear models for D_{LL}^B and D_{LL}^E. The left column of Figure

370   4 shows the residuals, defined as the difference between the model and satellite-derived $\log_{10} D_{LL}$

371   (referred to as the residuals), for both the train and test datasets (red and blue) and both D_{LL}^B and D_{LL}^E

372   (top and bottom). For both D_{LL}^B and D_{LL}^E the residuals are normally distributed and peak around zero for

373   both test and train data sets (left column). This is ideal as it demonstrates that in general the modelled

374   D_{LL}s are similar to the satellite-derived D_{LL}s. Further, the similarity in the distributions of train and test

375   residuals indicates that the model does not suffer from overfitting (e.g., fitting only to the training data).
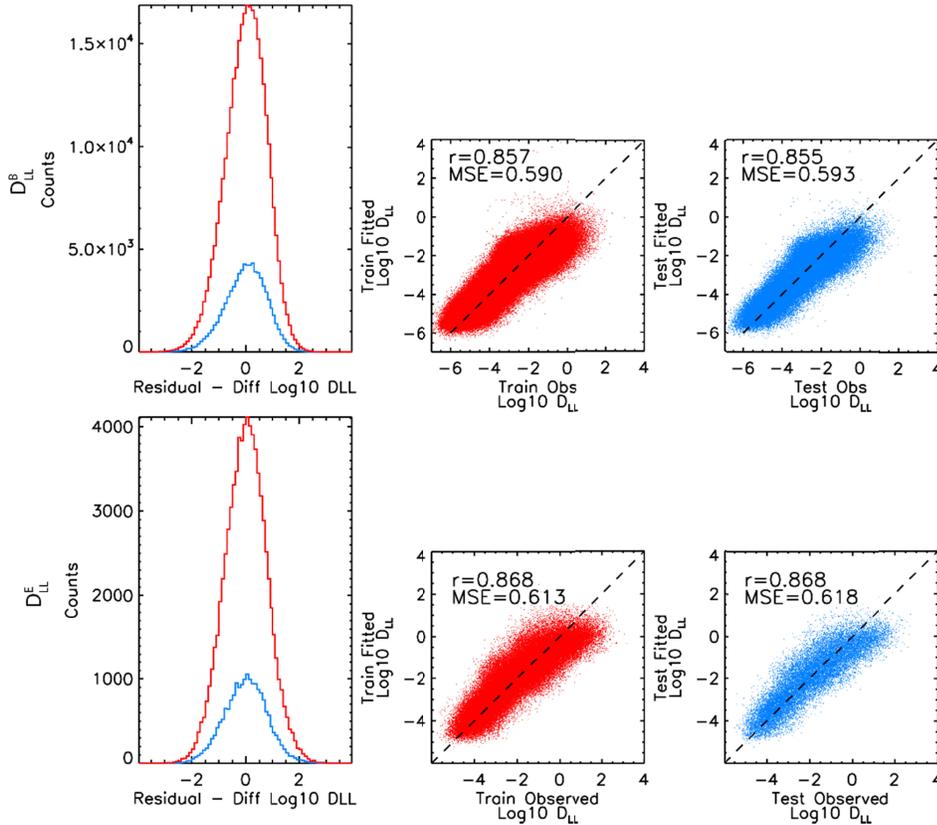
376

377   Figure 4: The residuals for the multi-linear regression D_{LL}^B and D_{LL}^E models (top and bottom). Right, distribution of

378   the residuals for the train and test data sets (red and blue). Middle and right, observed D_{LL} versus modelled D_{LL}

379   for the train and test data sets (blue and red); in each panel the correlation, r, and MSE are shown in the top left.

380   The middle and right columns of Figure 4 show the observed D_{LL} versus the modelled D_{LL} for both the

381   train and test datasets (middle and right); the correlation and MSE are shown in the top left. For both

382   D_{LL}^B and D_{LL}^E the correlation between the modelled and observed D_{LL}s in both the train and test data

383   sets is high, ~0.86 accounting for ~74% of the variance within the data sets. For both models the MSE is
384   also low. Overall, the normal distribution of the residuals, high correlation and low MSE, coupled with
385   the similarities between the train and test data sets demonstrates the robustness and accuracy of the
386   trained models. Table S2, shows the fitting and normalization coefficients for both D_{LL} models as
387   described by Equations 1 and 2.

3.3 Model Performance

389   In this section we investigate the residuals as a function of each independent variable to provide the
390   reader and specifically modelers with a clear overview of the model's performance under varying
391   conditions. Figure 5 shows the probability distribution functions (PDFs) of the D_{LL}^B and D_{LL}^E model
392   residuals (top and bottom; modelled D_{LL} minus satellite-derived D_{LL}) as a function of the independent
393   variables (rows) for the combined train and test datasets. In general, both the D_{LL}^B and D_{LL}^E models
394   perform well as a function of the independent variables. The residuals are peaked around zero as a
395   function of the independent variable. However, this is not true for L^* and for more extreme values of
396     $Sym\text{-}H$, B_z, and P_{dyn}. With regard to L^*, both the D_{LL}^B and D_{LL}^E models show bias at $L^* > 6$ and $L^* < 4.5$
397   where the residuals are skewed to either positive or negative values. The biases in L^* are more
398   pronounced than those observed as a function of $Sym\text{-}H$, B_z, and P_{dyn} and are likely the result of biases
399   that exist in in the calculation of L^*. Note, a similar distribution of residuals is observed when
400   considering only storm-time or quiet-time periods with this choice of independent variables. This
401   similarity is ideal as it demonstrates that both the D_{LL}^B and D_{LL}^E radial diffusion models perform well
402   during both storm- and quiet-times. This was not the case for storm- and non-storm-time Kp-
403   parameterisation of D_{LL} examined by Dimitrakoudis (2022) which highlights another pitfall of
404   parametrizing D_{LL} by Kp as such parameterizations cannot account for both storm and quiet times. Due
405   to the similarity between storm-time, quiet-time, and all data, the storm- and quiet-time distributions
406   are shown in Supporting Information S3 and S4.

13
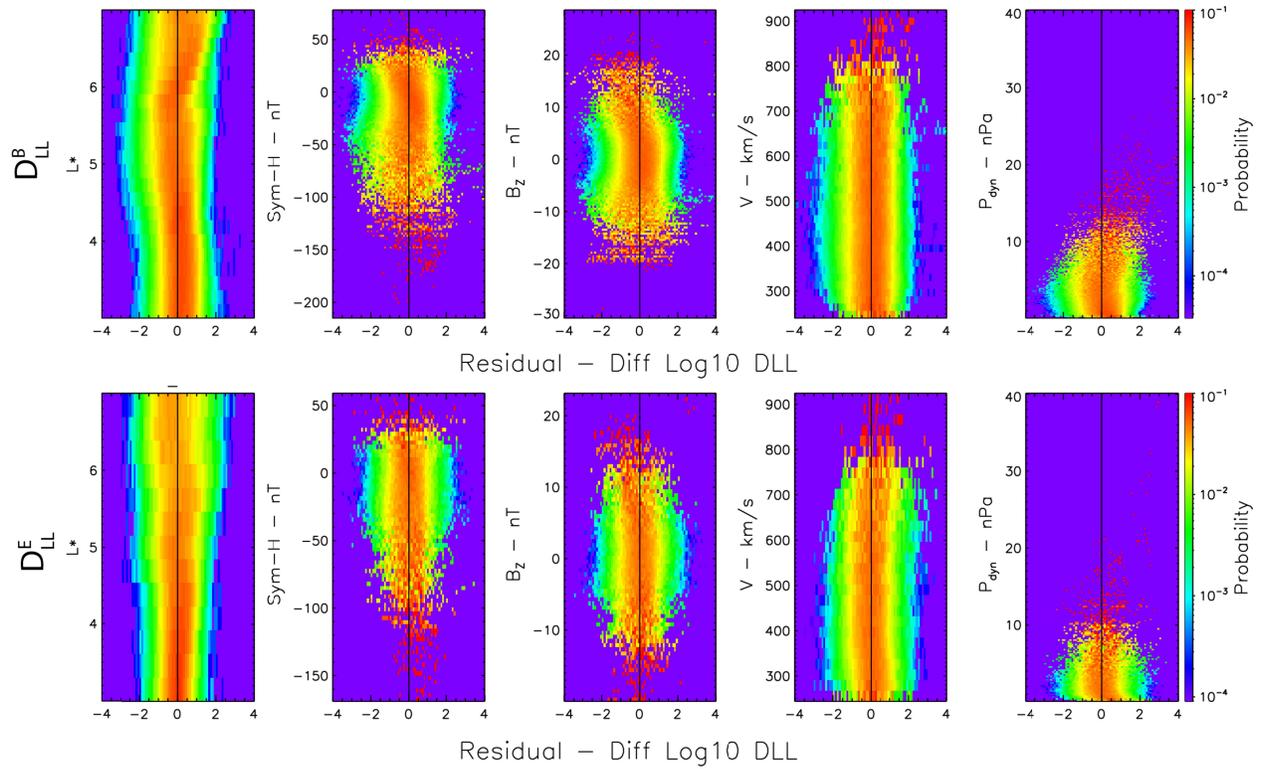
Figure 5: PDFs of the D_{LL}^B and D_{LL}^E model residuals calculated from the combined train and test data sets for each of the independent variables.

While the overall performance of both the D_{LL}^B and D_{LL}^E diffusion model is good (Figure 4) the biases as a function of L^* may introduce errors which can propagate through any radiation belt simulation. For this reason, the residuals have been characterized as a function of L^* so that the bias can be readily removed from the models. To remove the bias, we use the residual-L^* PDF. The data is binned in L^* in increments of 0.1 (corresponding to the grid size in many radiation belt simulations) and so are the residuals. For each L^* bin we fit a Gaussian of the form shown in equation 3, where A_0 is the height, A_1 is the center, and A_2 is the width (standard deviation) of the fitted Gaussian. This analysis is shown in Supporting Information Figure S5 for both the D_{LL}^B and D_{LL}^E models and several select L^* bins. From these fits we can use A_1 to shift the modelled D_{LL}s by subtracting A_1 from the modelled D_{LL} corresponding to a particular L^* bin. In this way when the residuals are recalculated they peak around zero.
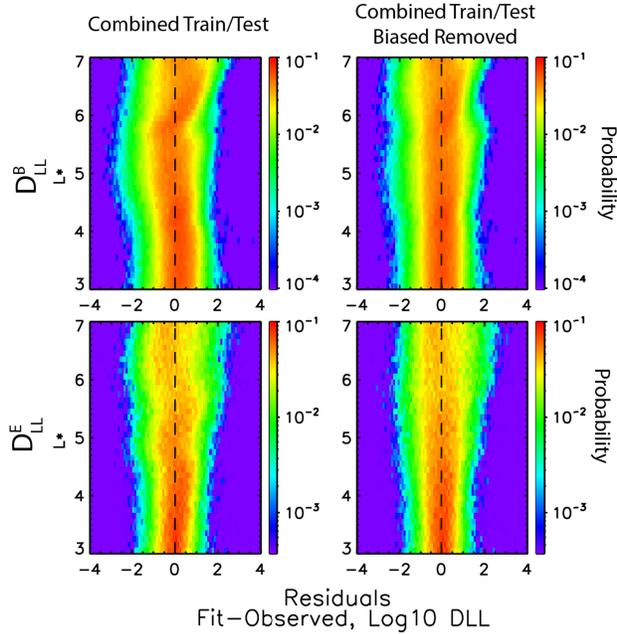
$$f(r) = A_0 e^{(\frac{r-A_1}{A_2})^2} \quad (3)$$

Figure 6: Comparison of the PDFs of both D_{LL}^B (top) and D_{LL}^E (bottom) model residuals (left) and residuals-biased-removed (right) of the combined train/test datasets

Figure 6 shows the results of the biased-removed D_{LL}s calculated by shifting each D_{LL} based on the Gaussian fits and corresponding L^* bin. The left column shows the PDF of residuals versus L^* and the right column shows the PDF of the residuals-biased-removed versus L^* for the combined trained/test datasets. Evident in Figure 6 is that once the bias is removed from the modelled D_{LL}s the residuals peak around zero and the bias as a function of L^* is no longer evident. In this analysis it is important to note that bias as function of L^* is discrete and not continuous; however, the bias has been characterized on an L^* grid typically used in radiation belt simulations. Finally, though not the purpose of characterizing residuals, the Gaussian fits provide a very simple means to generate ensembles of D_{LL}s which can be used in radiation belt simulations. For example, the width and center of the Gaussian can be used with a random number generator to sample from the fitted distribution of residuals and subtract the randomly sampled residual from the modeled D_{LL}s. In this way several D_{LL} time series can be generated to run ensemble simulations of the radiation belt response. Supporting Information Table S6 contains the Gaussian fit parameters as a function of L^* for both D_{LL}^B and D_{LL}^E. Note that the shift in the residuals, defined by the center of the Gaussian is largest for D_{LL}^B and that the D_{LL}^E model performs better then the D_{LL}^B. Finally, while these corrections help with the model residuals, they are generally small, not exceeding a factor of ~2.

4   Event Case studies and Model Comparisons

In the previous section we discussed the development of new D_{LL}^B and D_{LL}^E models and assessed their overall performance as a function of each independent variable. In this section we investigate the dynamics and performance of the new D_{LL}^B and D_{LL}^E models during two case studies, an extended period of quiet geomagnetic activity and the March 2013 Geospace Environment Modeling Quantitative Assessment of Radiation Belt Modeling focus group storm challenge event (e.g., Engebretson et al., 2018; Ma et al., 2018). For both cases we compare the D_{LL}s derived here with the Ozeke et al. (2014),

15

448 Brautigam and Albert (2000), and Lejosne (2019) D_{LL}s. Note the Ozeke et al. (2014), Brautigam and
449 Albert (2000), and Lejosne (2019) D_{LL}s are all parameterized by L and not L^*; however, since such
450 models are routinely used in simulations with no conversion to L^* we are able to compare them to the
451 model developed here assuming their L is directly used as L^* in simulations.
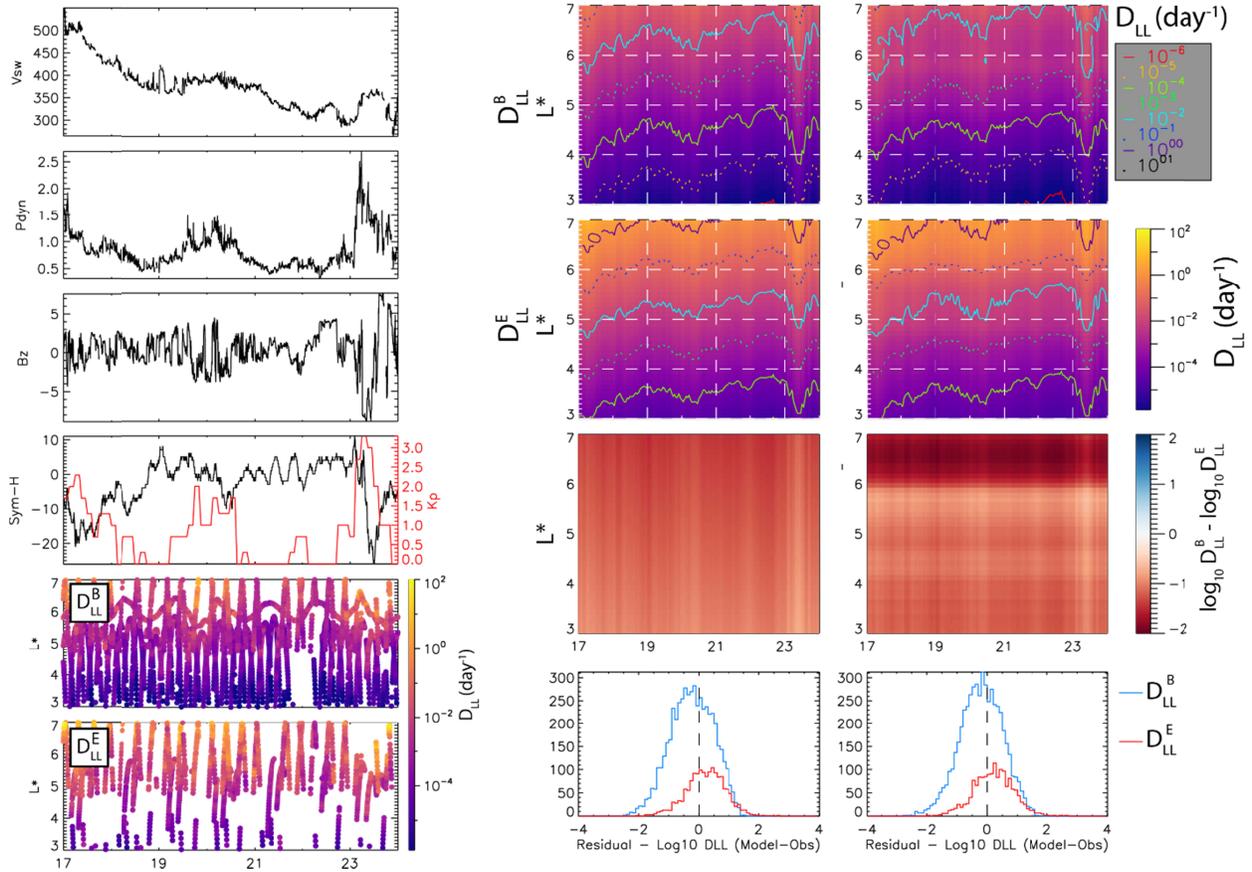
452

453 Figure 7: The modelled D_{LL}s during an interval of quiet solar wind and low geomagnetic activity. From top to
454 bottom the left panel shows V, P_{dyn}, B_z, $Sym\text{-}H$ (black) and Kp (red), and the satellite derived D_{LL}^B and D_{LL}^E. The
455 middle and right panel show the modelled and model-bias-removed D_{LL}s. From top to bottom the two right panels
456 show D_{LL}^B, D_{LL}^E, the difference between the log of D_{LL}^B and D_{LL}^E, and then the model residuals calculated by
457 comparing the modelled D_{LL}s to the satellite derived D_{LL}s. The contours in the top two panels are contours of
458 constant D_{LL}, the white dashed lines are placed at major tick marks to aid in comparison between the model and
459 model-bias-removed D_{LL}s.

460 Figure 7 provides an overview of the solar wind and geomagnetic conditions as well as the satellite-
461 derived D_{LL}s during a quiet solar wind and geomagnetic period in November 2013 (see caption for
462 details). At the start of the quiet period the solar wind speed was elevated and $Sym\text{-}H$ slightly negative
463 for ~12 hours. Towards the end of the interval the IMF turned southward in association with a period of
464 enhanced dynamic pressure and another period of negative $Sym\text{-}H$ lasting ~24 hours. Throughout the
465 quiet interval Kp remained low, below 3+. The observed D_{LL}s were largest at the start and end of the
466 quiet period, in association with elevated solar wind speeds and enhanced dynamic pressure and
467 southward IMF. Through the middle of the quiet period the observed D_{LL}s were generally small. This
468 can be seen in the bottom two rows of the left panel. Throughout the quiet period the modelled D_{LL}s

16

469 (middle and right panels) showed the same overall pattern as the observed D_{LL}s and the modelled
470 residuals remained consistent with the overall model performance (bottom panels of middle and right
471 column). There is also little difference between the modeled D_{LL}s and the modeled-biased-removed
472 D_{LL}s through the duration of the quiet period. Finally, in both models D_{LL}^E is larger then D_{LL}^B by about an
473 order of magnitude; this is generally consistent with the difference between D_{LL}^E and D_{LL}^B for higher
474 energy electrons in Ozeke et al. (2014).
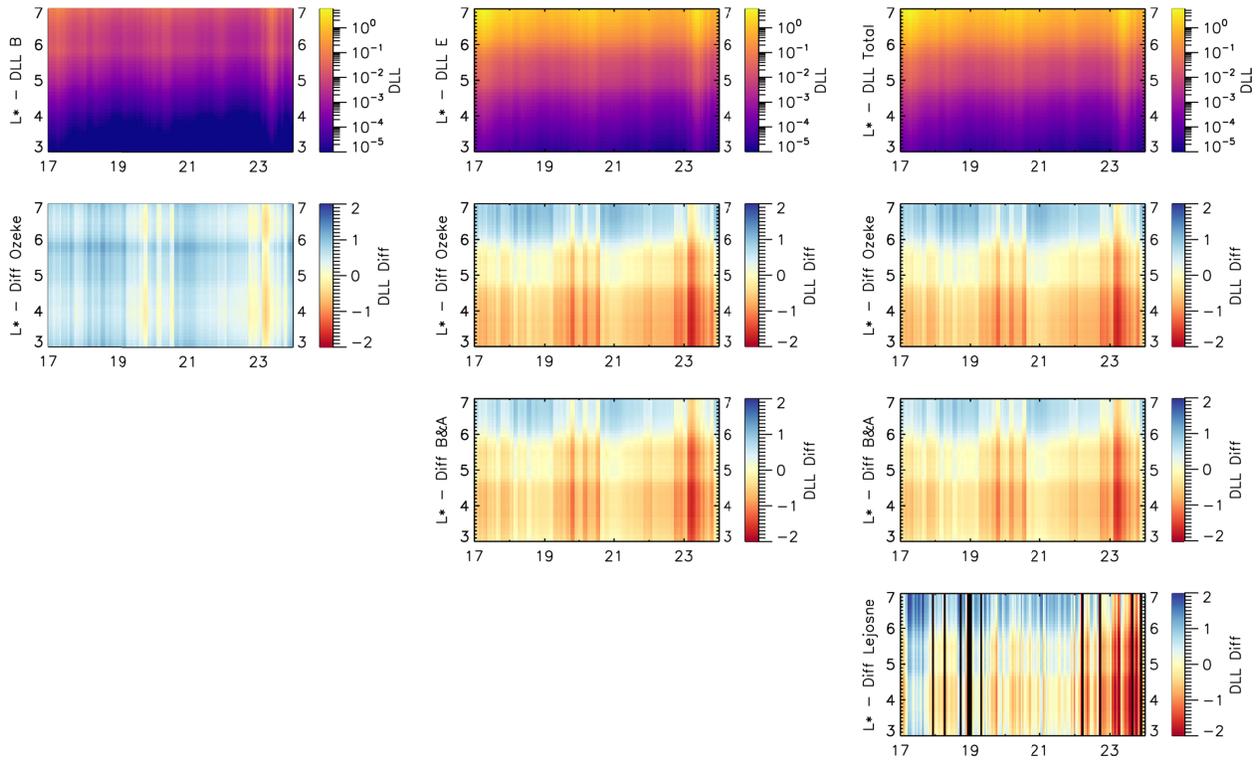
Figure 8: A comparison of bias-removed D_{LL}s derived here and those from Ozeke et al. (2014), Brautigam and Albert (2000), and Lejosne (2019). From left to right the columns show D_{LL}^B, D_{LL}^E, and $D_{LL}^T = D_{LL}^B + D_{LL}^E$. From top to bottom the rows show the modelled D_{LL}s derived here followed by the difference between the logs of modelled D_{LL}s and those from Ozeke et al. (2014), Brautigam and Albert (2000), and Lejosne (2019).

During the quiet interval the modelled D_{LL}s vary as one would expect. They were highest during elevated solar wind speed and negative $Sym\text{-}H$, and again with southward IMF, increased P_{dyn}, and negative $Sym\text{-}H$. However, what is more interesting, is the comparison between the D_{LL}s derived here and existing models of D_{LL}s (Figure 8). The top row of Figure 8 shows the modelled D_{LL}^B, D_{LL}^E, and the total $D_{LL}^T = D_{LL}^B + D_{LL}^E$, with the biases-removed. The subsequent rows show the difference between the logs of the model bias-removed D_{LL}s and the Ozeke et al. (2014), Brautigam and Albert (2000), and Lejosne (2019) D_{LL}s (see Figure caption for additional details). Compared to Ozeke et al. (2014), the modeled D_{LL}^B derived here is larger while the modeled D_{LL}^E derived here is larger at higher L^* and smaller at lower L^*. The combined diffusion D_{LL}^T shows the same pattern as D_{LL}^E. For Brautigam and Albert (2000) we only consider their electromagnetic term as the electrostatic term is typically ignored in radiation belt simulations (Ozeke et al. 2013). In this case the electromagnetic diffusion is larger than D_{LL}^E at higher L^* and smaller at lower L^*; the modelled D_{LL}^T shows the same pattern when compared to

492 the Brautigam and Albert (2000) electromagnetic term. A similar pattern is also observed when
493 comparing with the Lejosne (2019) D_{LL}s. In this case we only compare D_{LL}^T to those of Lejosne (2019) as
494 there is no analogous D_{LL}^E or D_{LL}^B. Note the Brautigam and Albert (2000) electromagnetic term and
495 Ozeke et al. (2014) D_{LL}^E are very similar in magnitude.

496
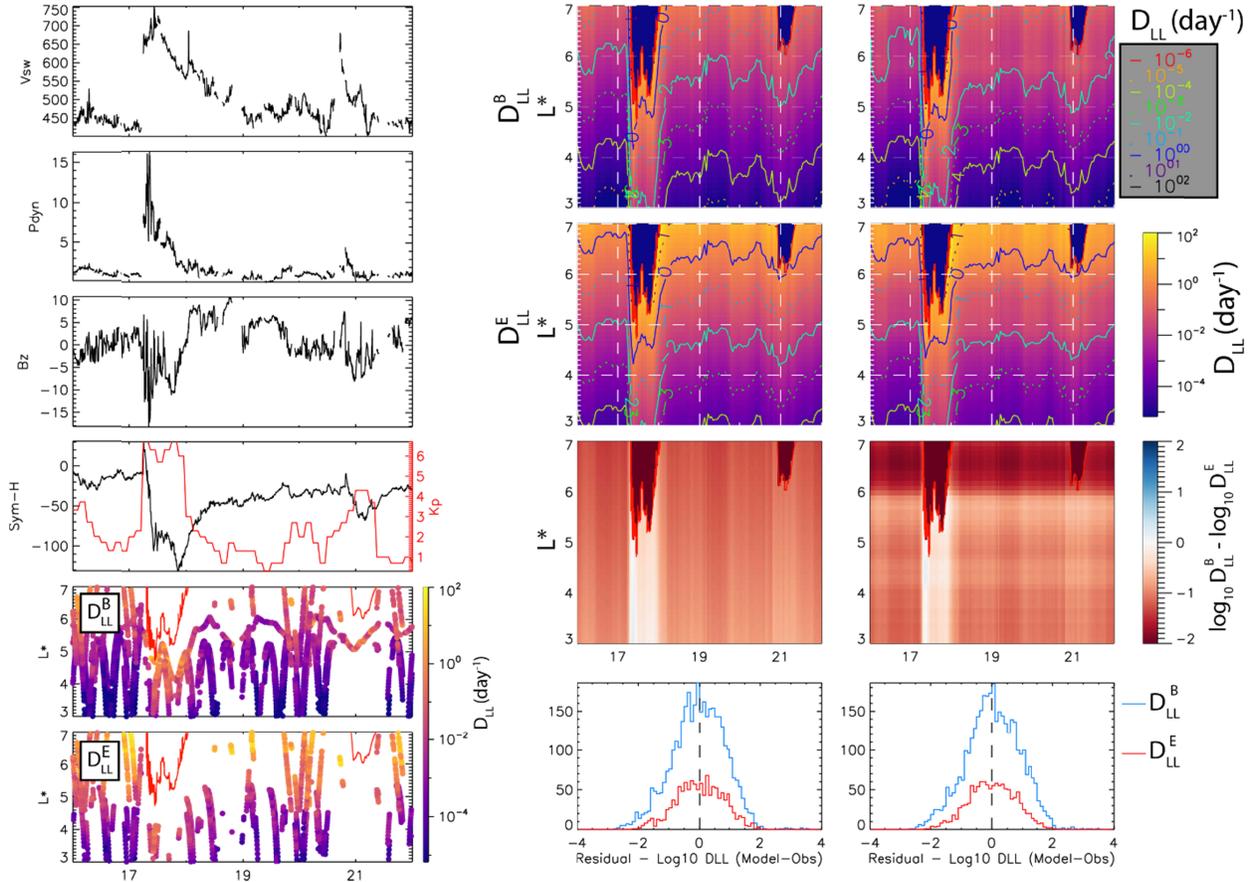
Figure 9: Solar wind dynamics, geomagnetic activity, satellite derived D_{LL}s, and modelled D_{LL}s during a geomagnetic storm in March 2013. The figure is in the same format as Figure 7. The red traces in the bottom two panels of the left column and top two panels of the middle and right column show the position of the last close drift shell throughout the interval.

501 Figure 9 and Figure 10 show the same set of observations, model-data comparison, and model-model
502 comparison as Figure 7 and Figure 8 for the March 2013 storm. The storm is associated with high-speed
503 solar wind, and ~1 day of large dynamic pressure and southward IMF (left panel Figure 9). This leads to a
504 large geomagnetic storm where the last closed drift shell reaches below geosynchronous orbit (red trace
505 in Figure 9 and Figure 10), Kp exceeds 6, and Sym-H reaches nearly -150 nT. During the main phase of
506 the storm, March 17, D_{LL}^B peaks and even exceeds D_{LL}^E during the same interval. This is consistent with
507 other studies which have shown D_{LL}^B to be large during the main phase of storms (Olifer et al., 2019;
508 Sandhu et al., 2021). Following the main phase and through the recovery phase both D_{LL}^B and D_{LL}^E decay
509 reaching pre-storm levels before rapidly enhancing again on March 21 during a second interval of fast
510 solar speed and southward IMF. These patterns are seen in the satellite-derived, modelled, and
511 modelled-biased-removed D_{LL}s (left, right and middle panels) and are consistent with what would be

512 expected given the solar wind and geomagnetic activity. Comparing the modelled and modelled-bias-
513 removed D_{LL}s there is generally little difference. The model bias-removed D_{LL}^B is slightly smaller at high
514 and low L^*. During the main phase $D_{LL}^B \approx D_{LL}^E$ in both models. Finally, the residuals for both models are
515 normally distributed and peak around zero.
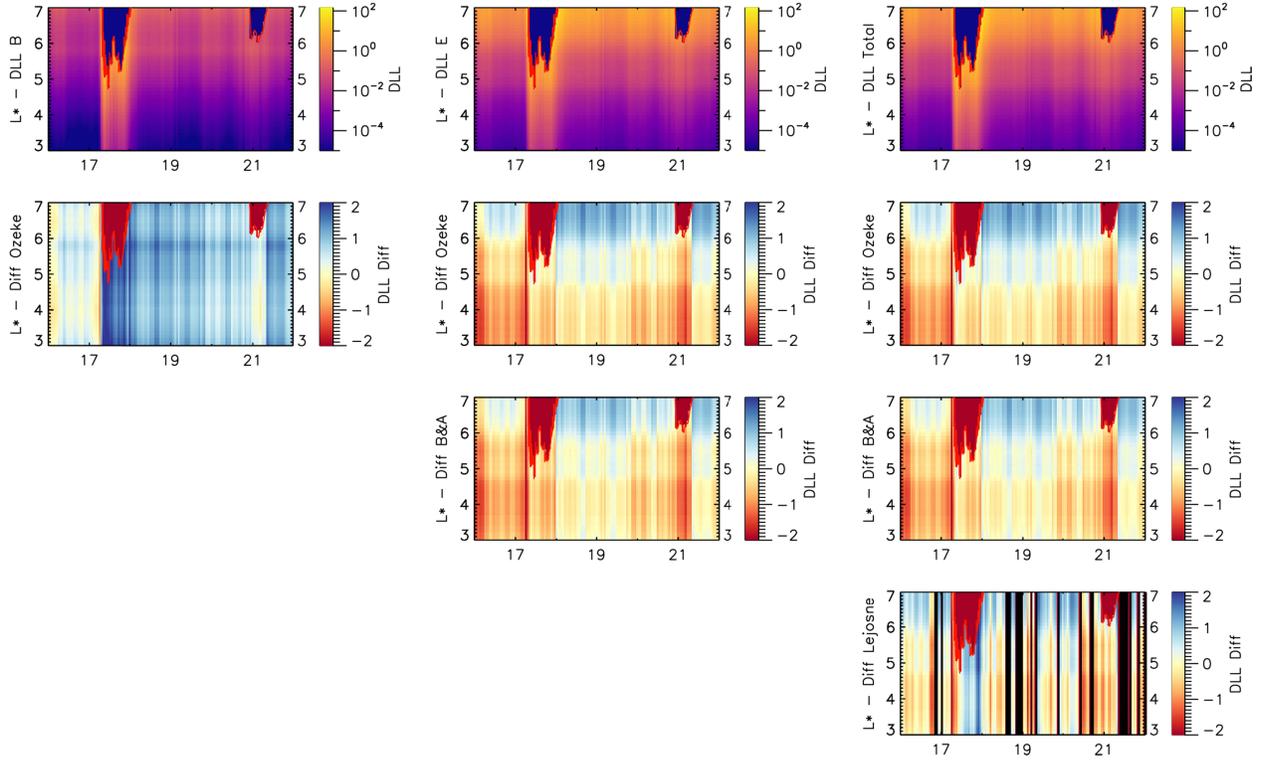
516

517 Figure 10: A comparison of the bias-removed D_{LL}s derived here and those from Ozeke et al. (2014), Brautigam and
518 Albert (2000), and Lejosne (2019) during a geomagnetic storm in March 2013. The figure is in the same format as
519 Figure 8. The red lines show the position of the last close drift shell throughout the interval.

520 During the geomagnetic storm (Figure 10) the D_{LL}s derived here show a similar relation to the Ozeke et
521 al. (2014), Brautigam and Albert (2000), and Lejosne (2019) D_{LL}s as that observed during quiet times
522 (Figure 8). D_{LL}^B is larger than that of Ozeke et al. (2014), especially during the main phase of the storm
523 (Figure 10 left). At high L^*, D_{LL}^E is larger than that of Ozeke et al. (2014) and Brautigam and Albert (2000)
524 and smaller at low L^* (Figure 10 Figure 10 middle). Comparing D_{LL} total (column 3) the D_{LL}s derived
525 here are larger at higher L^* and smaller at lower L^* as compared to Ozeke et al. (2014) and Brautigam
526 and Albert (2000) (Figure 10 right). Compared to Lejosne (2019) the D_{LL}s derived here are larger during
527 the main phase of the storm and at higher L and are generally smaller at lower L^* (Figure 10 bottom
528 right). Prior to the storm main phase, March 16, D_{LL}^E and D_{LL} total derived here are smaller then the
529 other three models across all L^*. During this period Kp is elevated compared to quiet values reaching a
530 Kp of 4, while the solar wind remains quiet accounting for the differences between the models.

531 # 5   Summary and Conclusions
532 In this work we utilize in-situ observations to develop a database of ULF wave power spectral density
533 (PSD) and satellite-derived ULF wave radial diffusion coefficients, D_{LL}s. The database of satellite-derived

534 D_{LL}s is used to construct a new L^* dependent and optimized bias-removed model of D_{LL}^B and D_{LL}^E driven

535 by B_z, V_{sw}, P_{dyn} and $Sym\text{-}H$. Overall, the new models of D_{LL}^B and D_{LL}^E perform well when compared to

536 the satellite-derived D_{LL}s from which the models were developed.

537 The new bias-removed D_{LL}s derived where compared to existing D_{LL} models from Ozeke et al. (2014),

538 Brautigam and Albert (2000), and Lejosne (2019) during a period of quiet geomagnetic activity and the

539 March 2013 geomagnetic storm. If one ignores the main phase of the storm, the comparison of quiet

540 time D_{LL}s is similar to that of the geomagnetic storm; D_{LL}^T generally has a steeper gradient as compared

541 to existing models such that D_{LL}^T is larger at high L^* and smaller at low L^*. The steeper gradient in the

542 D_{LL}s derived here is likely due to the use of a L^* and the TS05 model. The previous studies all used

543 dipole L which does not vary with varying solar wind and geomagnetic conditions. Whereas with L^*, as

544 activity increases the Earth's magnetic field is distorted resulting in changes in L^*. For example, during

545 periods of enhanced solar wind and geomagnetic activity regions of high ULF wave power can be

546 associated with lower L^* then would be in a dipole model; this leads to a steeper gradient in ULF wave

547 power as a function of L^* then as a function of L. Overall, the steeper gradient here is likely to be more

548 representative of the actual radial diffusion as it accounts for variations in the third adiabatic invariant

549 L^*.

550 During the main phase of the storm D_{LL}^T is larger then D_{LL} Lejosne (2019) and smaller then the Ozeke et

551 al. (2014), Brautigam and Albert (2000) D_{LL}s. And, prior to the storm onset, the D_{LL}s derived here are

552 smaller at all L^* values then the existing models. These differences are likely a result of the

553 parameterization used to quantify the D_{LL}s. Lejosne (2019) uses the magnetopause boundary defined

554 by P_{dyn} and B_z to derive the magnetic field perturbations which drive radial diffusion. Both P_{dyn} and B_z

555 are elevated for only a short period of time compared to $Sym\text{-}H$ and V_{sw} which is likely why the D_{LL}s

556 derived here are larger then those of Lejosne (2019) during the main phase. With regard to the period

557 prior to storm onset, Kp is elevated as compared to $Sym\text{-}H$, B_z, V_{sw}, and P_{dyn} which is likely why the

558 Ozeke et al. (2014) and Brautigam and Albert (2000) D_{LL}s are larger then those derived here. These

559 periods of elevated Kp are associate with enhanced AE driven by magnetospheric substorms. Though

560 substorm activity leads to enhanced ULF waves in the form of short lived and irregular pulsations

561 (Jacobs et al., 1964), the actual enhancement in Kp is the result of the larger substorm bays (Cramoysan

562 et al., 1995) as opposed to ULF waves. Thus, its unclear whether this period would in fact lead to

563 enhanced radial diffusion as depicted by the Ozeke et al. (2014) and Brautigam and Albert (2000) D_{LL}s

564 as the resulting substorm-driven ULF wave activity is short lived. This difference is likely to propagate

565 through any radial diffusion simulation leading to significant differences in the strength of radial

566 transport and global topology of the radiation belt when using the different D_{LL}models.

567 Finally, it is important to note that D_{LL}^B, D_{LL}^E and total D_{LL} can reach rates greater then 10/day. Though

568 this is in agreement with other models, as illustrated in **Error! Reference source not found.** (see also

569 lifer et al., 2019; Sandhu et al., 2021), at these values the concept of radial diffusion will start to break

570 down as electrons would be moving inward on time-scales on the order of or shorter than a drift period.

571 In this regime coherent ULF wave-particle interactions may instead play an important role in the global

572 dynamics of the outer radiation belt (e.g., Murphy 2020; 2018). The effect that enhanced ULF wave

573 power, which leads to these large D_{LL}s, and the effect they have on outer radiation belt is an important

574 avenue of future research and which can be investigated with global models (Degeling et al., 2008, 2013,

575 2014; Komar et al., 2017).

576 In summary, we have used over 40 years of satellite data to calculate D_{LL}^B and D_{LL}^E over a range of L^*

577 from 3-7 in non-dipole field using TS05. The diffusion rates are parameterised by an optimized set of

578 solar wind and geomagnetic variables and provide diffusion coefficients at much higher time resolution

579 and over a larger dynamic range then previous studies. The main results are:

580 - The gradient in our D_{LL}^T is generally steeper as compared to existing models, giving higher
581   diffusion rates at larger L^* and lower rates at low L^*.
582 - D_{LL}^E is generally higher than D_{LL}^B at all L^* except during the main phase of storms.
583 - During the March 2013 magnetic storm D_{LL} generally agrees with previous work except for the
584   initial phase of the storm where diffusion rates are lower at all L* < 5. We suggest that this is
585   due to substorm activity which is captured in the Kp models and not in our new models.
586
587 The results are available for use in global radiation belt models to develop better reconstructions of the

588 radiation belt environment (see Supporting Information for model coefficients). Future work will test

589 both the model and model bias-removed D_{LL} performance in radiation belt simulations under varying

590 geomagnetic conditions to determine if the new models improve the performance of radiation belt

591 simulations as compared to existing D_{LL} models. In addition, future studies will investigate the

592 performance of our new models as compared to existing models when using forecasted inputs. Finally,

593 future studies will investigate including additional model inputs and independent variables and the time

594 history of independent variables, along with more complex algorithms for regression as a path to

595 improved D_{LL} models and radiation belt simulations.

Open Research

608 The THEMIS data is available via SPEDAS, PySPEDAS or the THEMIS data server,

609 http://themis.ssl.berkeley.edu/data/themis. The GOES data is available from the NOAA National Centers

610 for Environmental Information website, https://www.ngdc.noaa.gov/stp/satellite/goes/. Van Allen

611 Probes data is available at the Coordinated Data Analysis Web (CDAWeb) https://cdaweb.gsfc.nasa.gov/.

612   The OMNI data is available at https://omniweb.gsfc.nasa.gov/. The higher level database used to
613   develop the D_{LL} models is available via Zenodo, https://zenodo.org/record/7569732, doi:
614   10.5281/zenodo.7569732. The database contains two data sets, a magnetic field data set and an electric
615   field data set. The magnetic field dataset contains the derived power spectral density for the
616   compressional magnetic field $B_\parallel$ from THEMIS, Van Allen Probes, and accompanying position (MLT, L, L*
617   TS05), solar wind, and geomagnetic data. The electric field contains the derived power spectral density
618   for the azimuthal electric field E_φ from THEMIS, Van Allen Probes, and GOES and accompanying position
619   (MLT, L, L* TS05), solar wind, and geomagnetic data. See the Zenodo record for more description of the
620   derived database and datasets.

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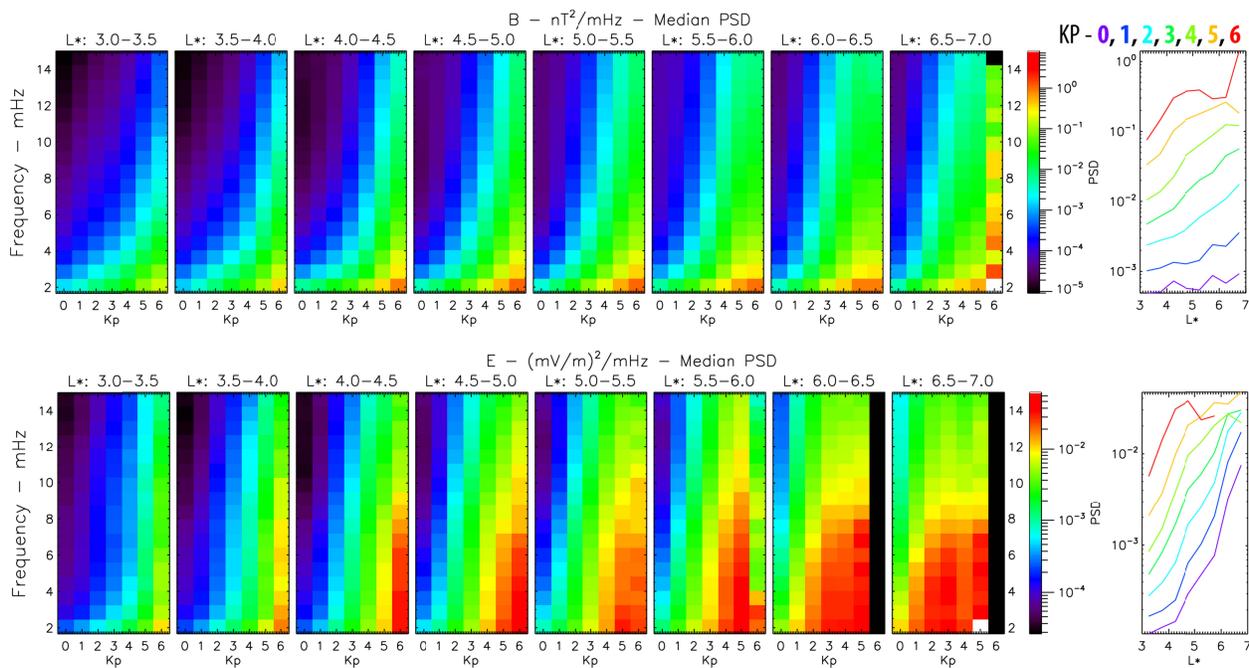
Figures

Figure 11: Statistical variation of the $B_\parallel$ (top) and E_φ (bottom) PSD. The spectral plots show the median PSD as a function of frequency (y-axis), Kp (x-axis) and L* (panels 1-8). The line plots show the variation of PSD at fixed a frequency of 2.5 mHz as a function of L* and Kp (color) for the entire dataset.
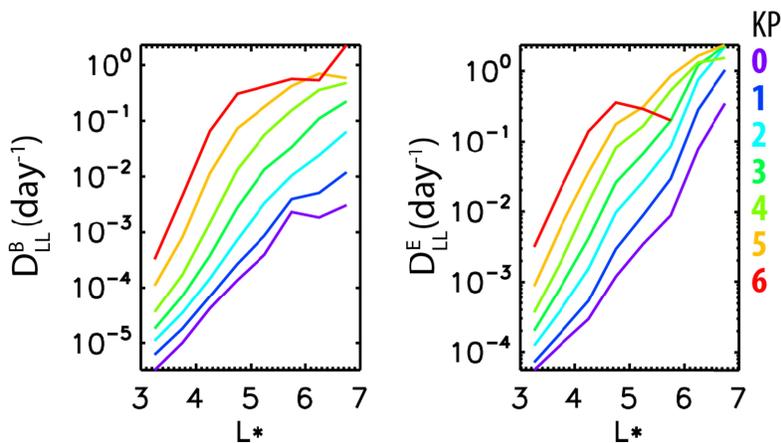
Figure 12: Median D_{LL}^B (left) and D_{LL}^E (right) as function of L* and Kp for the entire dataset.

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Figure 13: Results of the parametric study. (a) and (b) Correlation and mean square error (MSE) of data and multi-linear regression model for all combinations of independent variables (identified as integers on the x-axis). (c) A zoom in of (a) and (b) highlighting the combination of independent variables resulting in a high correlation and low MSE between the data and multi-linear regression model; the black line is the correlation and blue the MSE, the x-axis shows the various combinations of independent variables.

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Figure 14: The residuals for the multi-linear regression D_{LL}^B and D_{LL}^E models (top and bottom). Right, distribution of the residuals for the train and test data sets (red and blue). Middle and right, observed D_{LL} versus modelled D_{LL} for the train and test data sets (blue and red); in each panel the correlation, r, and MSE are shown in the top left.

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Figure 15: PDFs of the D_{LL}^B and D_{LL}^E model residuals calculated from the combined train and test data sets for each of the independent variables.
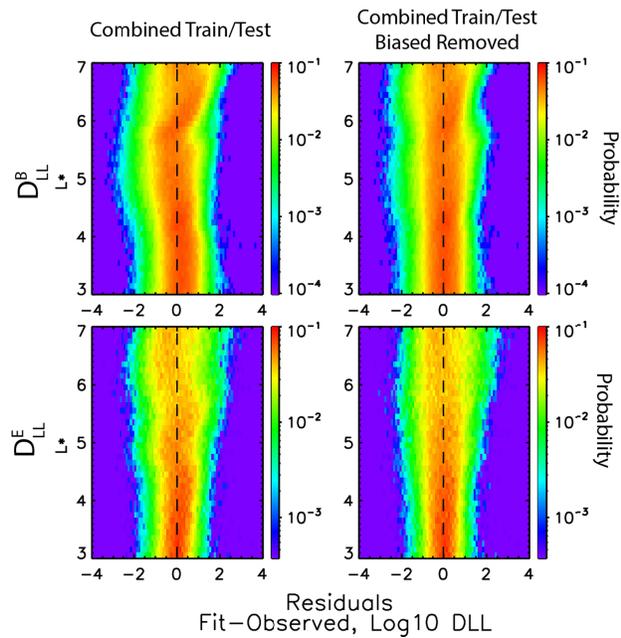
Figure 16: Comparison of the PDFs of both D_{LL}^B (top) and D_{LL}^E (bottom) model residuals (left) and residuals-biased-removed (right) of the combined train/test datasets

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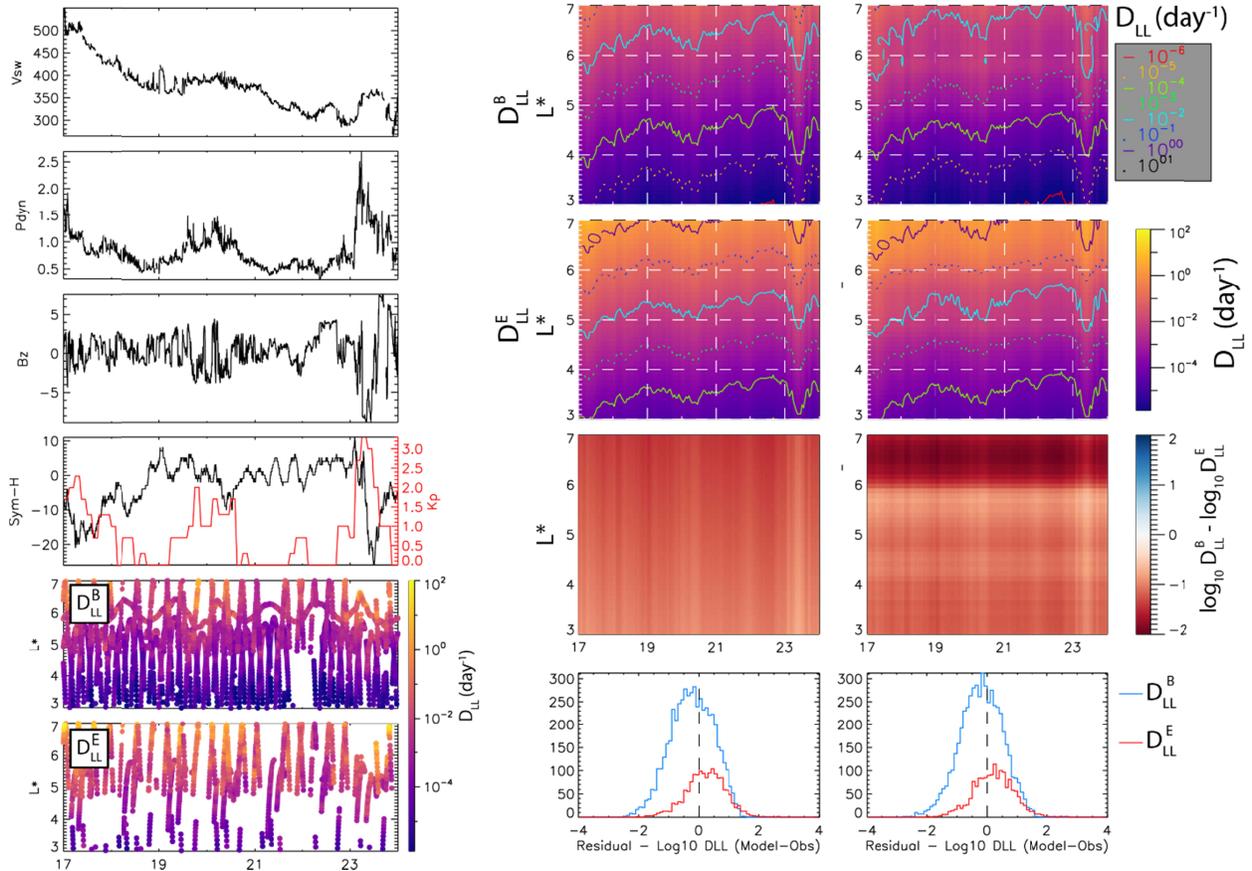
Figure 17: The modelled D_{LL}s during an interval of quiet solar wind and low geomagnetic activity. From top to bottom the left panel shows V, P_{dyn}, B_z, $Sym\text{-}H$ (black) and Kp (red), and the satellite derived D_{LL}^B and D_{LL}^E. The middle and right panel show the modelled and model-bias-removed D_{LL}s. From top to bottom the two right panels show D_{LL}^B, D_{LL}^E, the difference between the log of D_{LL}^B and D_{LL}^E, and then the model residuals calculated by comparing the modelled D_{LL}s to the satellite derived D_{LL}s. The contours in the top two panels are contours of constant D_{LL}, the white dashed lines are placed at major tick marks to aid in comparison between the model and model-bias-removed D_{LL}s.

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Figure 18: A comparison of bias-removed D_{LL}s derived here and those from Ozeke et al. (2014), Brautigam and
Albert (2000), and Lejosne (2019). From left to right the columns show D_{LL}^B, D_{LL}^E, and $D_{LL}^T = D_{LL}^B + D_{LL}^E$. From top to
bottom the rows show the modelled D_{LL}s derived here followed by the difference between the logs of modelled
D_{LL}s and those from Ozeke et al. (2014), Brautigam and Albert (2000), and Lejosne (2019).

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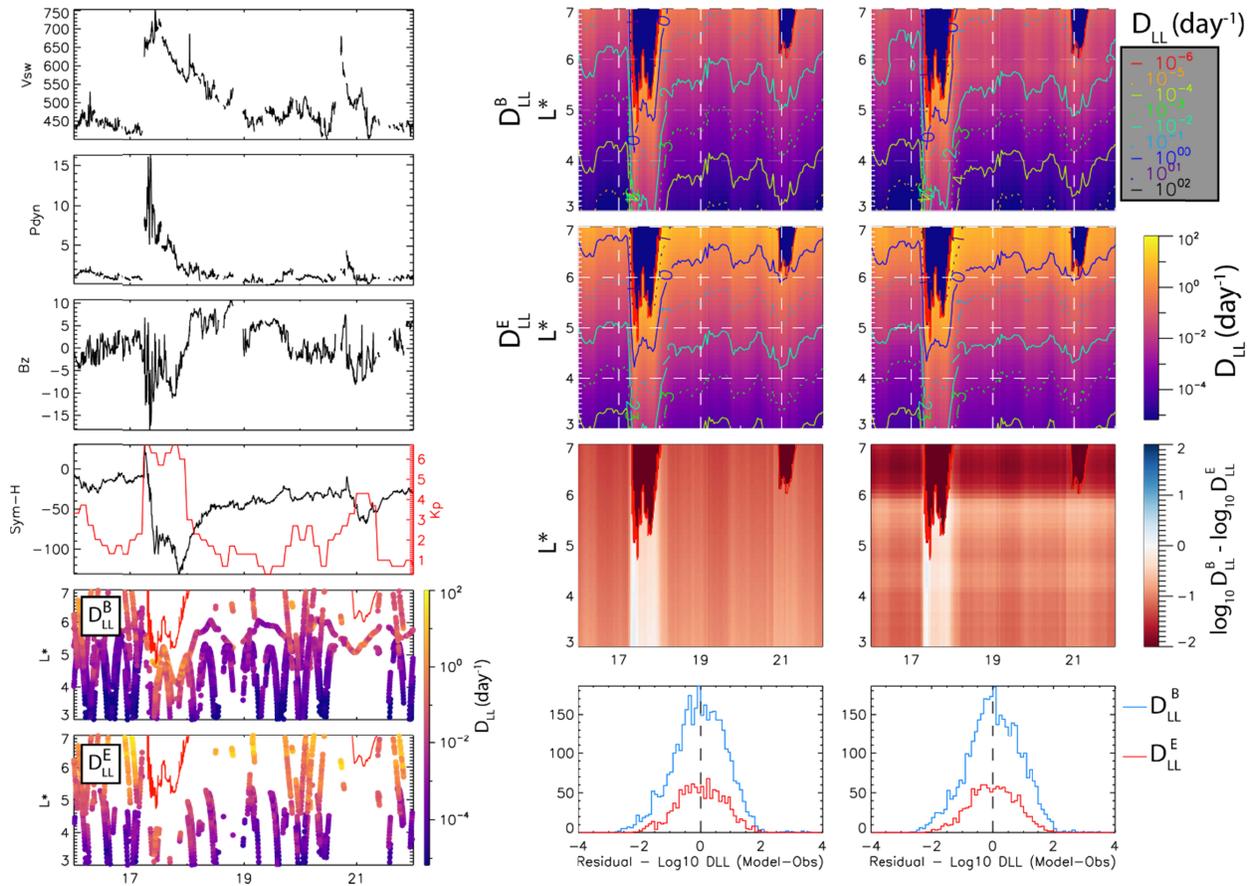
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666 Figure 19: Solar wind dynamics, geomagnetic activity, satellite derived D_{LL}s, and modelled D_{LL}s during a
667 geomagnetic storm in March 2013. The figure is in the same format as Figure 7. The red traces in the bottom two
668 panels of the left column and top two panels of the middle and right column show the position of the last close
669 drift shell throughout the interval.

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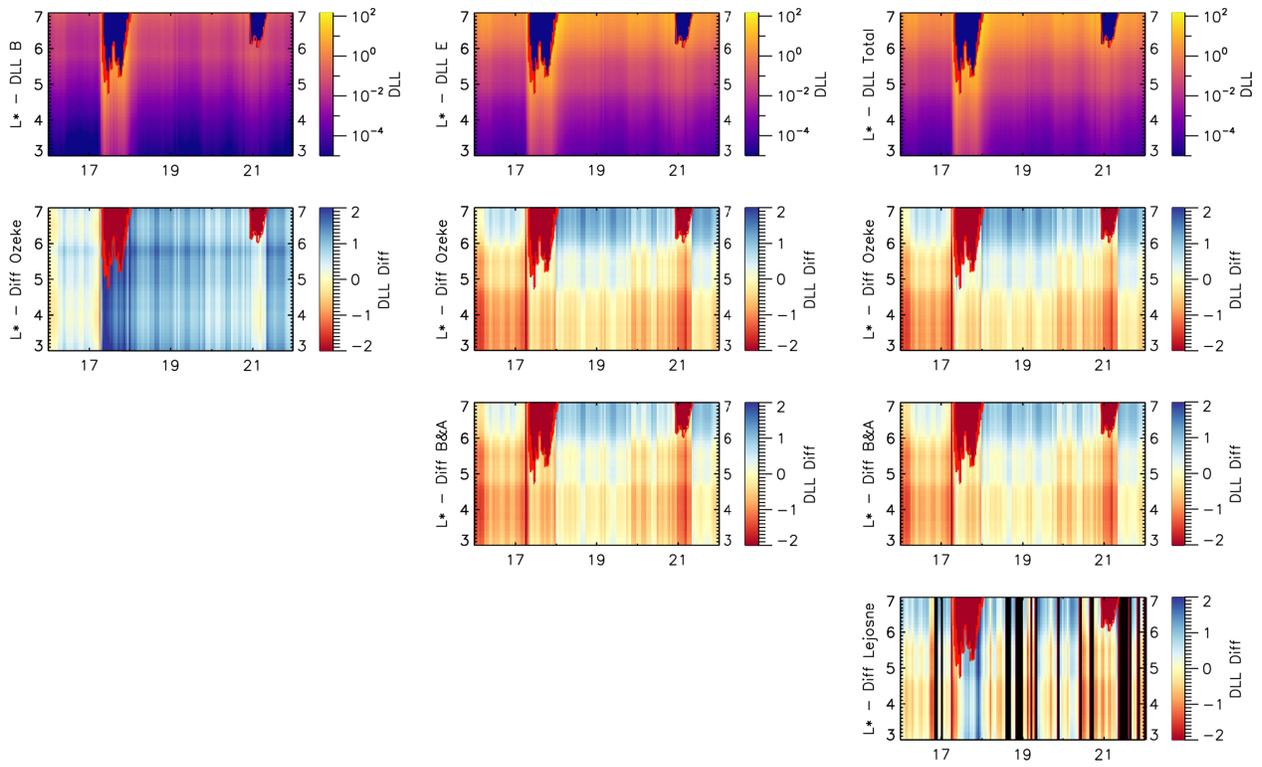
Figure 20: A comparison of the bias-removed D_{LL}s derived here and those from Ozeke et al. (2014), Brautigam and Albert (2000), and Lejosne (2019) during a geomagnetic storm in March 2013. The figure is in the same format as Figure 8. The red lines show the position of the last close drift shell throughout the interval.

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911

Figure 1.

B − nT^2/mHz − Median PSD

E − (mV/m)^2/mHz − Median PSD

KP − 0, 1, 2, 3, 4, 5, 6

Figure 2.

Figure 3.

(a) (b) (c)

Figure 4.

Figure 5.

Figure axes (top row, D_{LL}^B): $L*$, $Sym-H - nT$, $B_z - nT$, $V - km/s$, $P_{dyn} - nPa$, with colorbar labeled Probability.

Figure axes (bottom row, D_{LL}^E): $L*$, $Sym-H - nT$, $B_z - nT$, $V - km/s$, $P_{dyn} - nPa$, with colorbar labeled Probability.
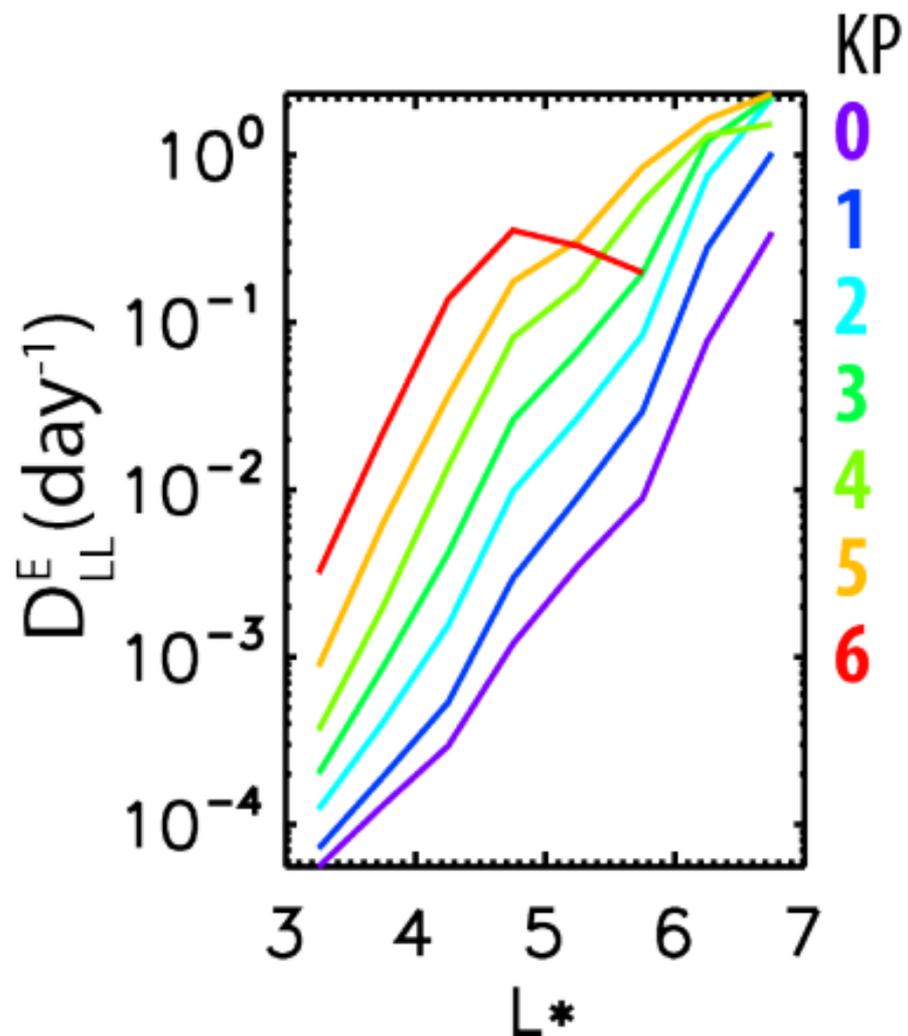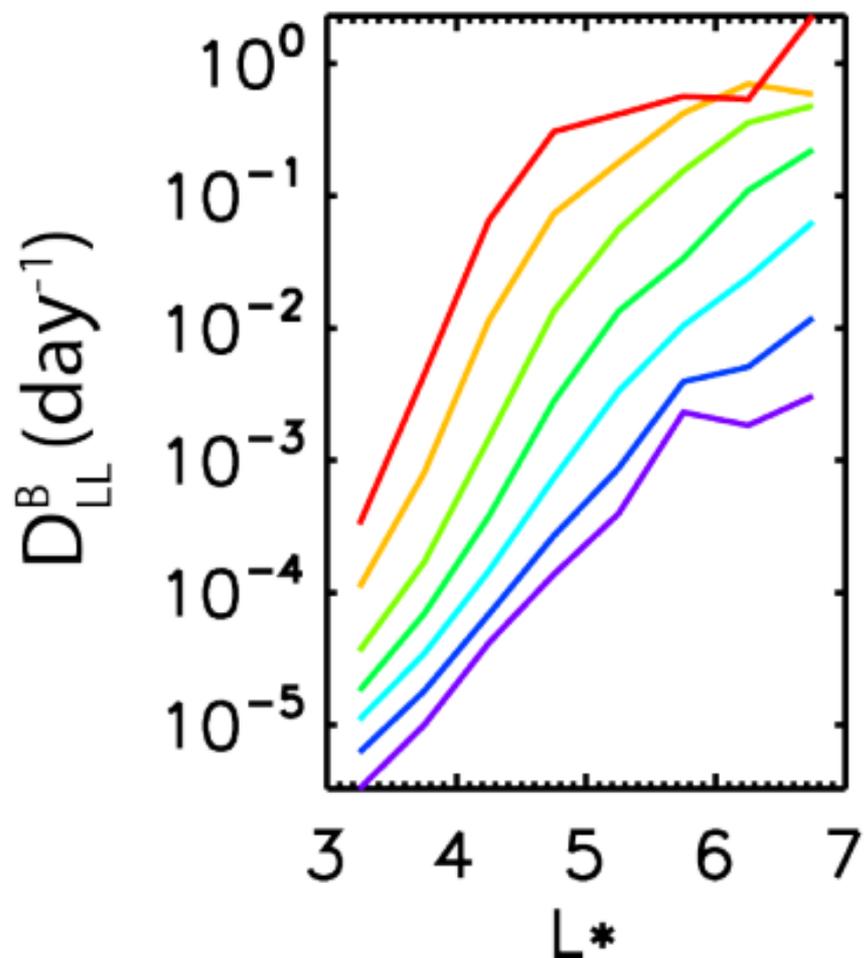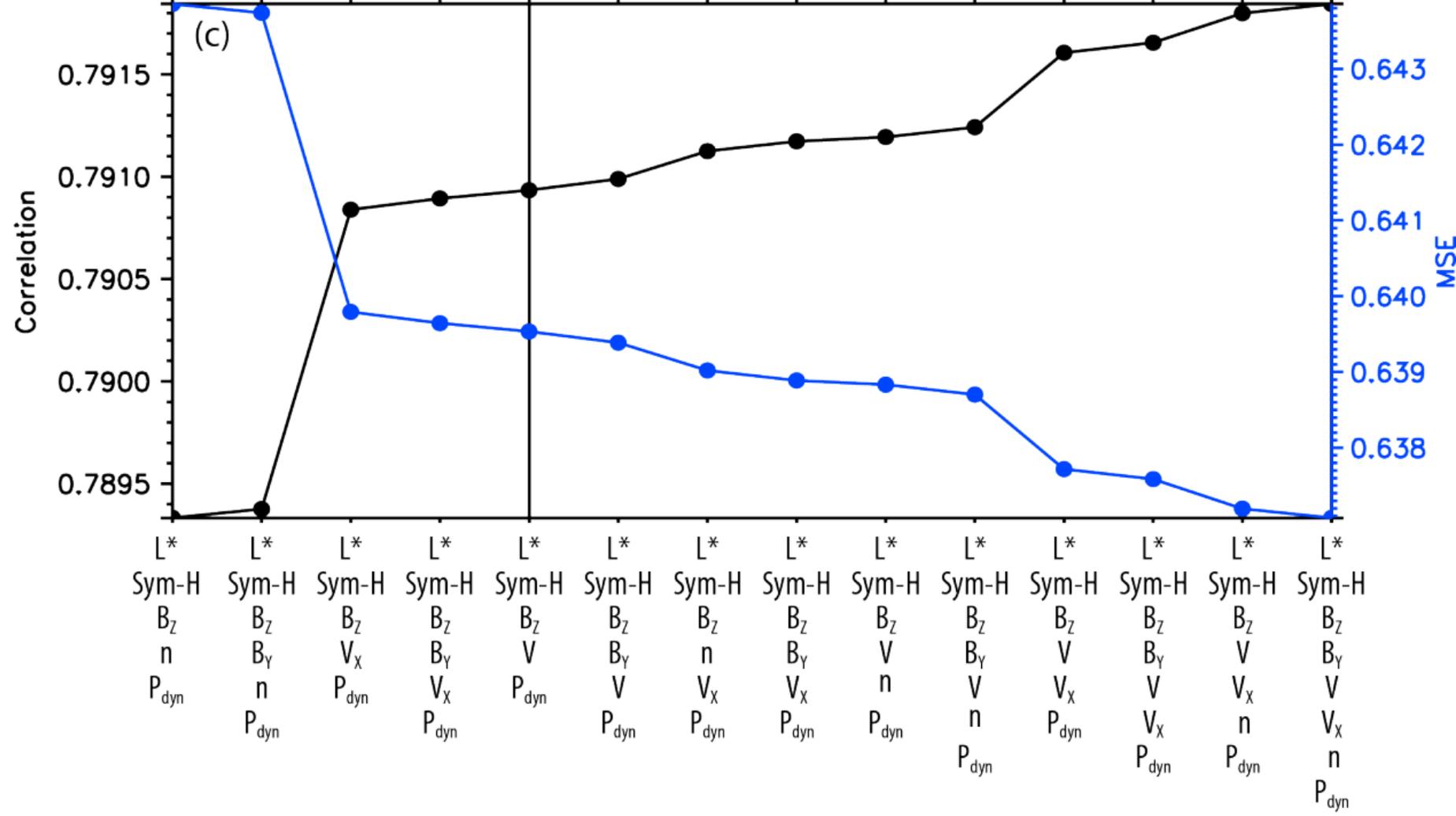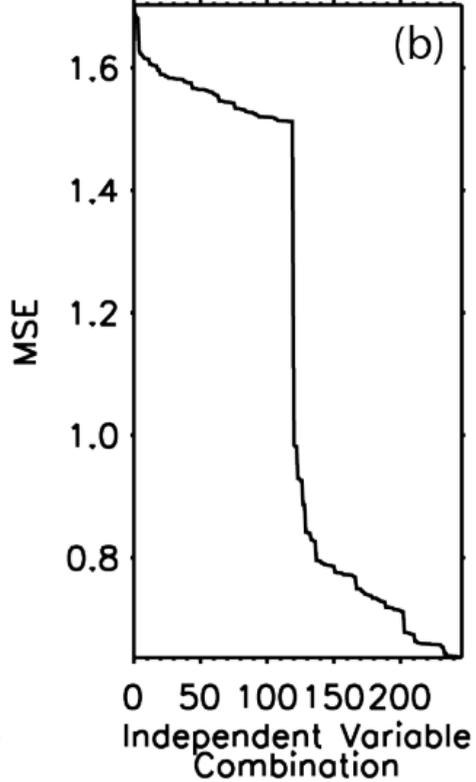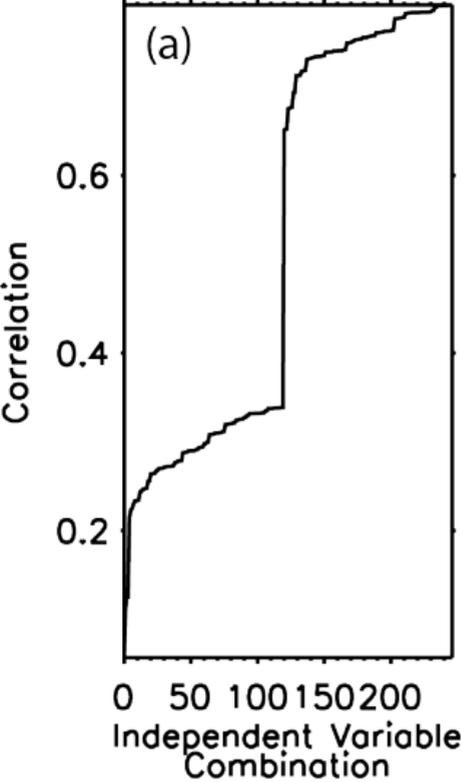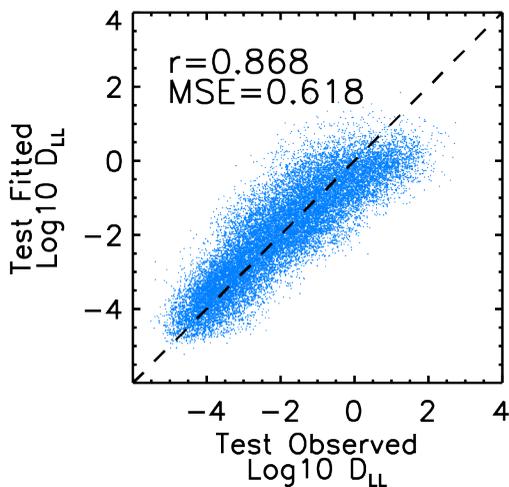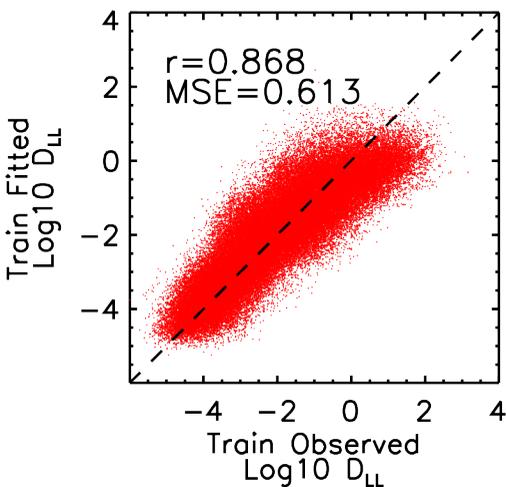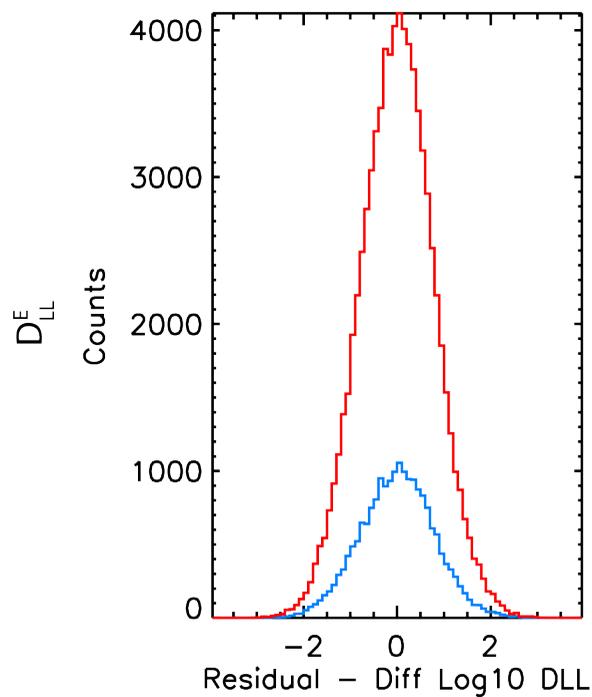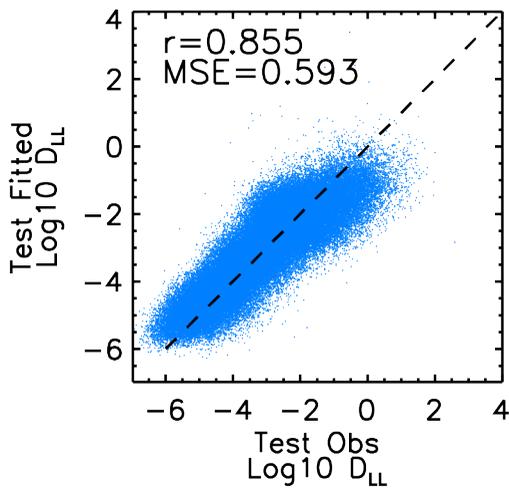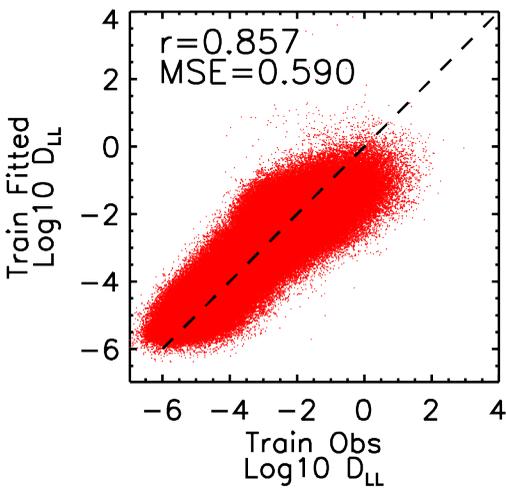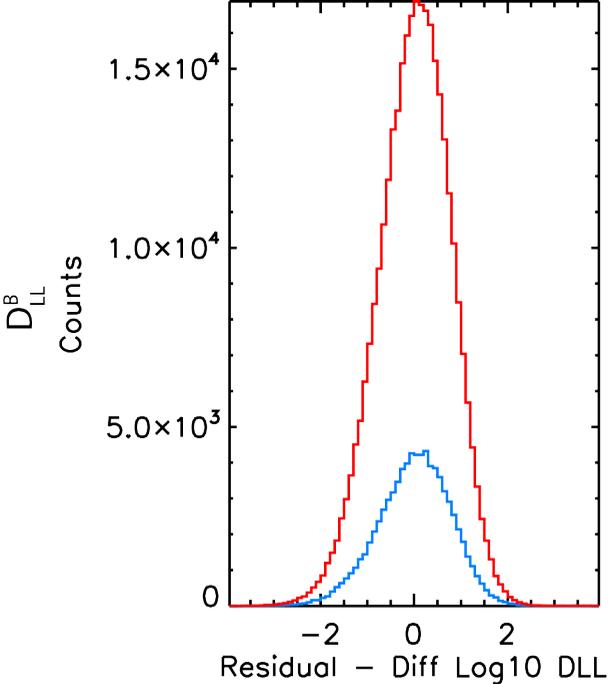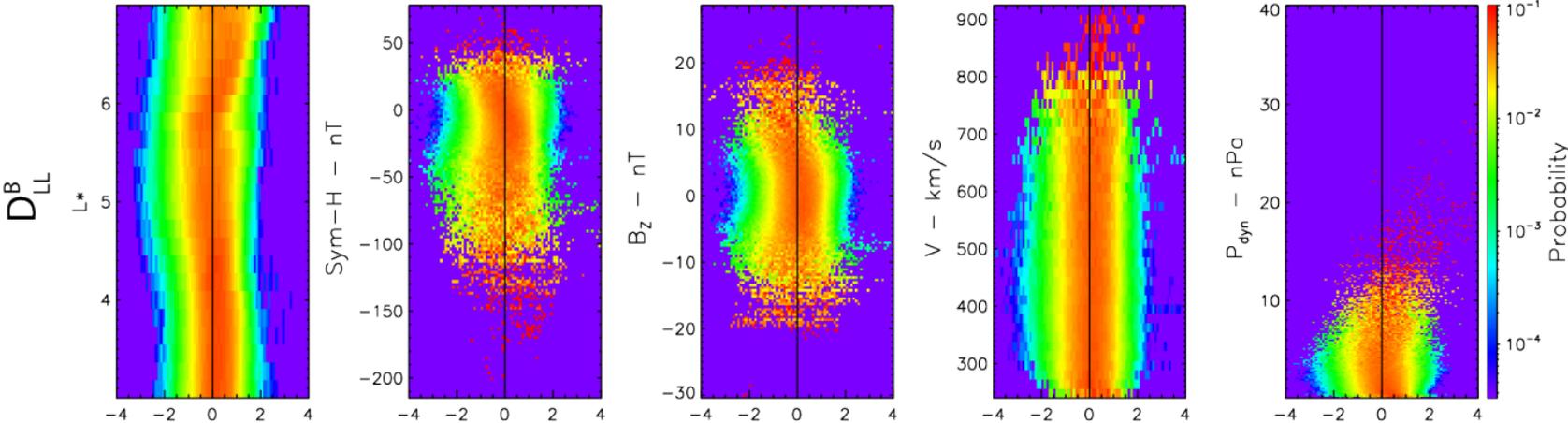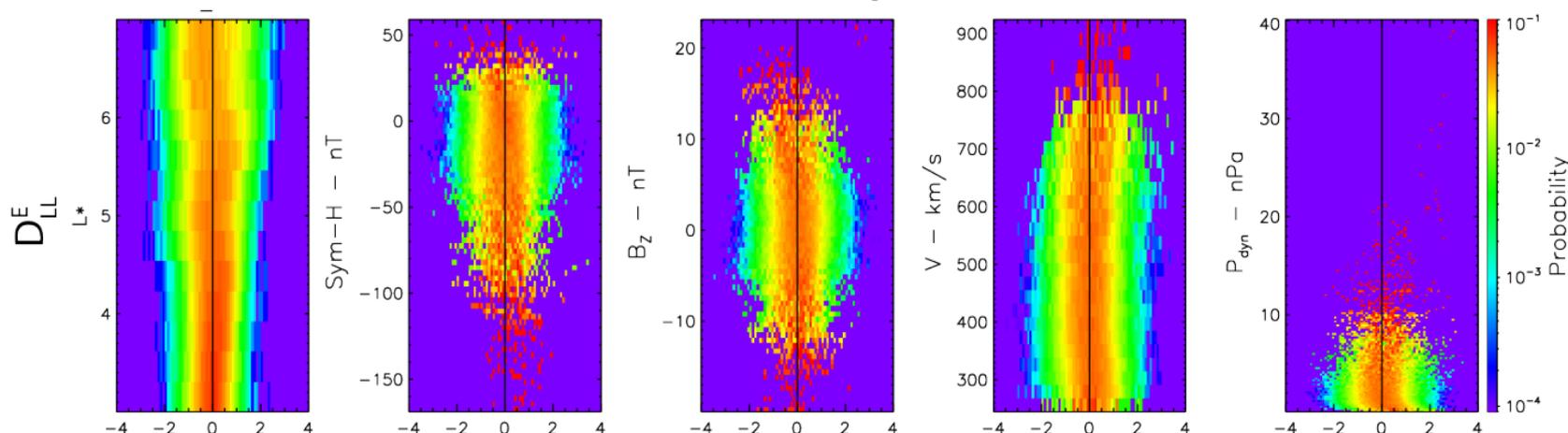
Residual − Diff Log10 DLL

Figure 6.

Combined Train/Test
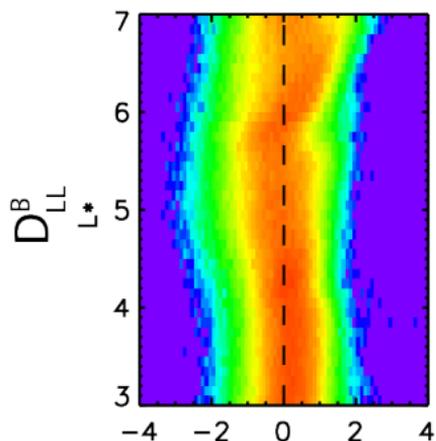
Combined Train/Test
Biased Removed

D^B_{LL}

D^E_{LL}

L*

Probability
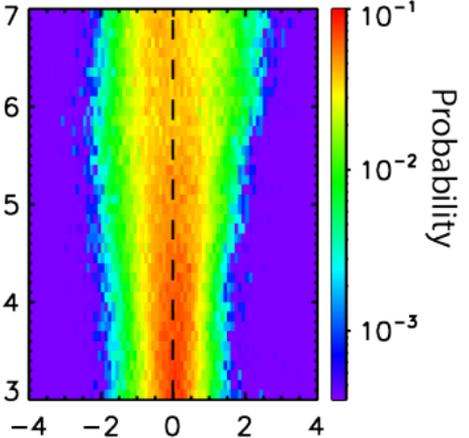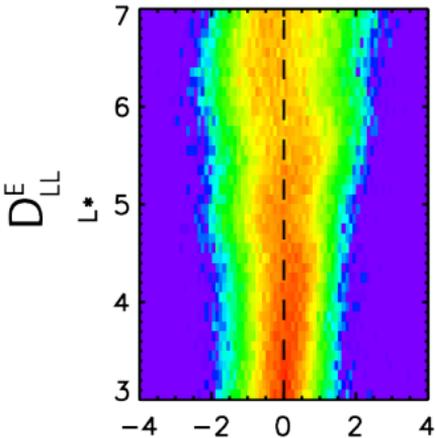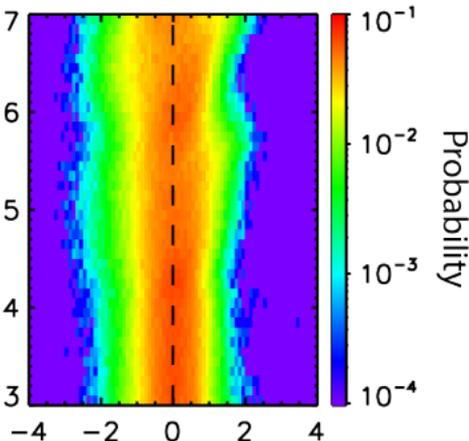
Residuals
Fit-Observed, Log10 DLL

Figure 7.
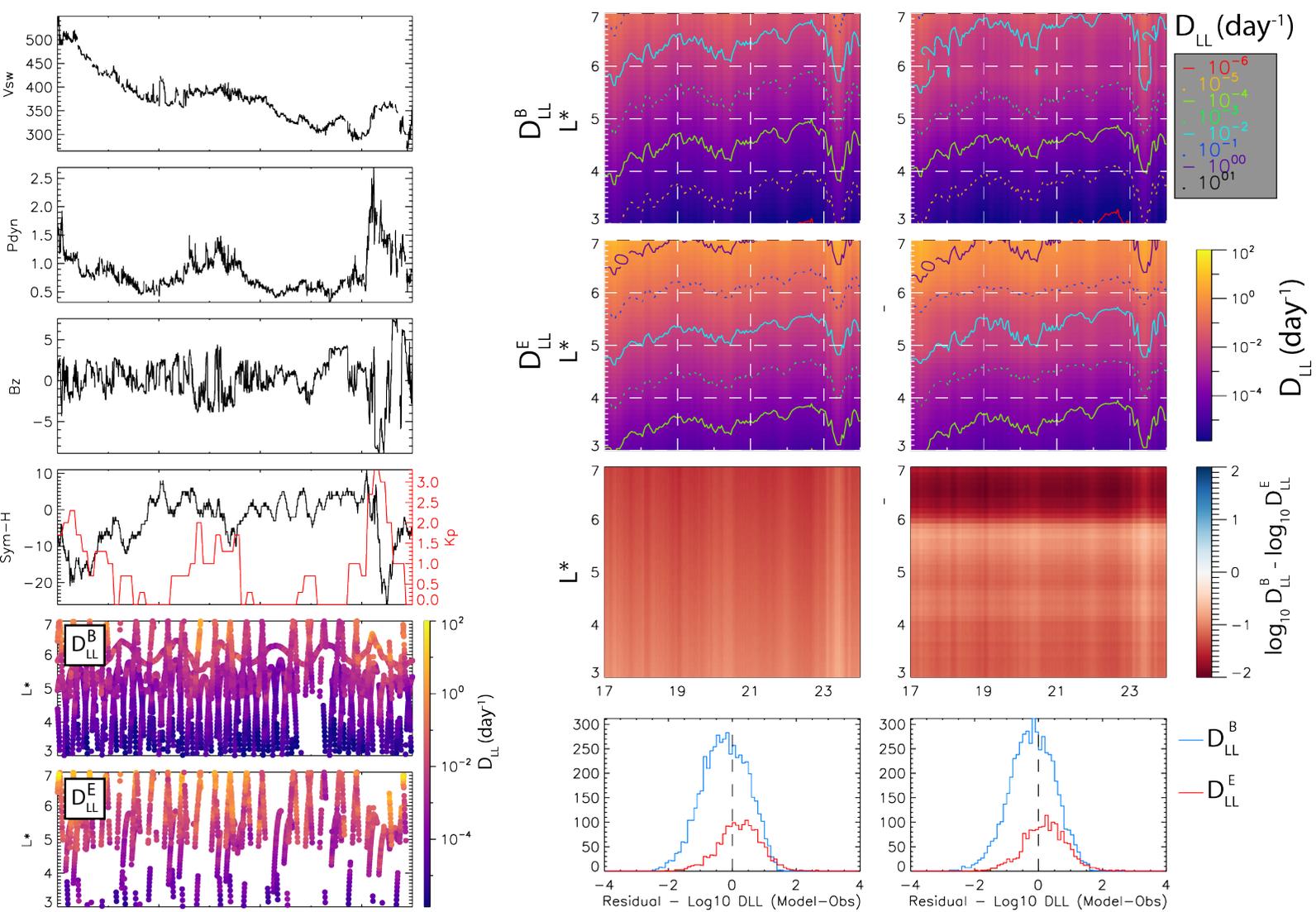
Figure 8.

Figure 9.

Figure 10.