- Modeling the magnetospheric X-ray emission from
- ² solar wind charge exchange with verification from

³ XMM-Newton observations

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Key Points.

- MHD based simulations provide a viable alternative to empirical modeling of X-ray emissivity.
- SWCX enhancement variance strongly depends on the accuracy of the heavy ion abundance.

Modeled X-ray emissivity provides global imaging of the magnetosheath.
Abstract. An MHD based model of terrestrial solar wind charge exchange

 $_{5}$ (SWCX) is created and compared to 19 case study observations in the 0.5-

 $_{\rm 6}$ $\,$ 0.7 keV emission band taken from the EPIC cameras on board XMM-Newton.

 $_{\scriptscriptstyle 7}~$ This model incorporates the GUMICS-4 MHD code and produces an X-ray

 $_{\circ}~$ emission datacube from ${\rm O}^{7+}$ and ${\rm O}^{8+}$ emission lines around the Earth using

⁹ in-situ solar wind parameters as the model input. This study details the modeling

¹⁰ process and shows that fixing the oxygen abundances to a constant value reduces

¹¹ the variance when comparing to the observations, at the cost of a small accuracy

¹² decrease in some cases. Using the ACE oxygen data returns a wide ranging

¹³ accuracy, providing excellent correlation in a few cases and poor/anti correlation

¹⁴ in others. The sources of error for any user wishing to simulate terrestrial

¹⁵ SWCX using an MHD model are described here and include mask position,

¹⁶ hydrogen to oxygen ratio in the solar wind and charge state abundances. A

¹⁷ dawn-dusk asymmetry is also found, similar to the results of empirical modeling.

¹⁸ Using constant oxygen parameters, magnitudes approximately double that

¹⁹ of the observed count rates are returned. A high accuracy is determined between

 $_{20}$ the model and observations when comparing the count rate difference between

²¹ enhanced SWCX and quiescent periods.

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1. Introduction

The terrestrial solar wind charge exchange process involves the liberation and capture 22 of an electron from a neutral species at the Earth (i.e., hydrogen) to a heavy, high 23 charge state, ion in the solar wind. The electron can be captured in an excited state and 24 transition to lower energy states via photon emission; which in the cases of X-ray photons, 25 is detectable by X-ray telescopes [e.g. Cravens et al., 2001; Henley and Shelton, 2008]. 26 X-ray charge exchange is a non-thermal emission, which was first detected in Röntgen-27 Satellit (ROSAT) observations of comets, when the solar wind interacted with the neutral 28 gas outflow [Lisse et al., 1996; Cravens, 1997]. Quantification of the X-ray emission has 29 focussed on highly ionised oxygen [e.g. Koutroumpa, 2012] as most space based X-ray 30 observatories investigate photon energies around $\frac{3}{4}$ keV and have observed SWCX in this 31 energy range, including XMM-Newton [e.g. Snowden et al., 2004], Suzaku [Ishikawa et al., 32 2013] and Chandra [Slavin et al., 2013]. More recent attempts at quantifying charge 33 exchange from other ions with emission lines around the $\frac{1}{4}$ keV band have also been 34 performed, though the lack of cross sectional information for a number of faint transition 35 lines causes a high uncertainty in the results [Kuntz et al., 2015]. This previous research 36 also showed a stronger correlation of the $\frac{1}{4}$ keV band ROSAT fluxes with solar wind flux 37 than the $\frac{3}{4}$ keV band. 38

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⁴⁰ Charge exchange emission has the possibility of being used as a powerful global imaging ⁴¹ tool [*Collier et al.*, 2012]. The peak charge exchange emission is expected to occur around ⁴² the subsolar magnetopause boundary where the pressure balance between the solar wind

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and terrestrial atmosphere sits, thus allowing magnetopause, neutral hydrogen and plasma 43 dynamics models to be tested using a global view rather than via traditional in-situ 44 measurements [Robertson et al., 2006; Collier et al., 2010]. An example of the clear 45 boundary definition can be seen in panel e) of Figure 1. The magnetopause can be seen at 46 a subsolar distance of $9R_E$, while the bow shock sits at around $11R_E$. The charge exchange 47 process has previously been used for magnetopause modeling, using the resultant energetic 48 neutral atom emission from low charge state ions [e.g., Collier et al., 2005; Hosokawa et al., 49 2008; Ogasawara et al., 2013]. Charge exchange X-ray emission has also been observed 50 at Venus [Dennerl, 2008], Mars [Holmström et al., 2001] and the Moon [Collier et al., 51 2014]. This indicates that for comparisons between the induced magnetospheres of the 52 unmagnetised planets and the Earth's magnetosheath, X-ray charge exchange emission 53 could be a valuable tool. This is especially true with magnetopause modeling as the 54 movement of the boundary layer provides a proxy for monitoring the transfer of solar 55 wind energy into the magnetosphere [Milan et al., 2004]. Hence, modeling and testing 56 of the terrestrial charge exchange process is necessary for understanding future imaging 57 studies. 58

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⁶⁰ The XMM-Newton observatory [Jansen et al., 2001] was launched in 1999 and currently ⁶¹ moves in a highly elliptical orbit with a perigee altitude of ~7000 km and an apogee of ⁶² ~114,000 km, allowing long observation periods (~48 hour orbital period with 42 hours of ⁶³ observations per orbit). The European Photon Imaging Camera (EPIC) onboard XMM-⁶⁴ Newton, contains two MOS CCD cameras [*Turner et al.*, 2001] and a single pn CCD ⁶⁵ camera [*Strüder et al.*, 2001], which provides a spectral resolution of $\frac{\Delta E}{E} \sim 17$. We use

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observations from the EPIC-MOS cameras in this study and all mention of EPIC data 66 refers to the MOS instruments. The EPIC-MOS cameras have a circular field of view 67 with a 30 arcminute (0.5°) diameter. While this field of view provides a high spatial 68 resolution at galactic distances, near the Earth this corresponds to ~ 60 km across the 69 camera. When we refer to SWCX we specifically mean the terrestrial emission. Our 70 main aim is to determine the efficacy of using a magnetohydrodynamic simulation, in 71 comparison to empirical models which have previously been used, to compare to observed 72 SWCX X-ray emission. Kuntz et al. [2015] showed that the Spreiter magnetopause model 73 [Spreiter et al., 1966], typically used in empirical modeling of SWCX, underestimates 74 the magnetopause position. We use an MHD model for this comparative study and a 75 more recent magnetopause model. To determine the properties of the solar wind plasma 76 throughout the magnetosheath we use the GUMICS-4 (Global Unified Magnetosphere-77 Ionosphere Coupling Simulation) MHD code [Janhunen et al., 2012]. The process to acquire and convert the MHD grid into an X-ray emissivity datacube is described in 79 Section 2. We then compare a line-of-sight integral through the datacube with the 80 observations made by the EPIC-MOS cameras in Section 3. Section 4 looks at improving 81 the correlation between observations and modeling, while Section 5 investigates the 82 influence of the oxygen related variables. We then provide our conclusions in Section 6. 83

2. Method

2.1. XMM-Newton EPIC observation cases

A sytematic identification of observations affected by SWCX has been previously determined for XMM-Newton up to revolution 1773 in August 2009 [*Carter et al.*, 2011]. These cases were found by searching for variability in the 0.5 to 0.7 keV band which

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is primarily made up of O^{7+} and O^{8+} emission lines. Comparison of this variability in 87 the oxygen $\frac{3}{4}$ keV band to the steady, source removed, continuum lightcurve of diffuse 88 emission in the 2.5 to 5.0 keV band can indicate SWCX when the correlations between 89 them are low [Carter and Sembay, 2008]. Table A.1 from Carter et al. [2011] lists 103 90 observations which are affected by SWCX in order of highest variability (χ^2_{μ}) between 91 the steady continuum and oxygen band. We have chosen the top 30 observations (not 92 including the comet cases), ranked by χ^2_{μ} from 27.2 to 3.4 as the basis for this study. 93 These cases are indicated as having the highest deviance between the X-ray background 94 flux and oxygen emission. Table 1 gives the revolution number and observation identifiers 95 for each of the selected cases, and we also include the date and the duration in hours. 96

2.2. Creating an X-ray emissivity cube

⁹⁷ To create an X-ray emissivity grid for each timestep in the MHD model we use ⁹⁸ Equation (1) [*Cravens*, 2000]. This requires the combination of the GUMICS-4 MHD ⁹⁹ simulation output with both the neutral hydrogen number density and the alpha value ¹⁰⁰ (α), a scale factor containing the cross section of the charge exchange interaction.

$$P_X = \eta_H \eta_{SW} v_{av} \alpha \tag{1}$$

¹⁰² where:

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¹⁰³ $P_X = \text{emissivity (eV cm}^{-3} \text{ s}^{-1})$

- $\eta_{SW} = \text{solar wind proton number density (cm}^{-3})$
- η_H = neutral hydrogen number density (cm⁻³)
- $\alpha = \text{scale factor based on cross sectional data and oxygen abundance (eV cm²)$

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¹⁰⁷
$$v_{av} = \sqrt{v_{sw}^2 + \frac{3k_BT}{m_p}} \quad (\text{cm s}^{-1})$$

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¹⁰⁹ 2.2.1. The GUMICS-4 MHD model

As a first step to running the MHD model we require the upstream solar wind conditions 110 as an input to the GUMICS-4 code. These solar wind parameters are downloaded from 111 NASA's Space Physics Data Facility in the form of OMNI [King and Papitashvili, 2005] 112 one minute resolution averages, a dataset taken from a combination of ACE, WIND and 113 IMP 8 satellite data, and timeshifted to the bow-shock. The required input variables 114 for GUMICS-4 are time (s), proton number density (m^{-3}) , temperature (°K), solar wind 115 speed (v_x , v_y , v_z in m/s), and interplanetary magnetic field (B_x , B_y and B_z in T). In order 116 to ensure a divergenceless solution, the IMF B_x component is kept constant. Missing data 117 values in the OMNI data set have a linear interpolation applied to recover appropriate 118 values for each timestep. We run the GUMICS-4 model using a four second timestep with 119 a data output grid produced every five minutes (300s). 120

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Once we have produced a set of MHD output datacubes for the duration of each XMM-Newton observation, we take a cuboid spatial subset covering the regions of interest (i.e., dayside magnetosheath). We define our irregular data grid with the highest spatial resolution closest to the planet, having limits of 0 to 15 R_E in GSE x and -18 to 18 R_E in GSE y and z in increasing intervals from 0.2 R_E up to 0.5 R_E . We use this grid in combination with the relevant GUMICS-4 output file to produce a datacube giving solar

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wind proton number density, velocity and temperature for each GSE x, y and z grid value.

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¹³⁰ 2.2.2. The neutral hydrogen model

We use the Hodges neutral hydrogen model [Hodges, 1994] to create a grid of neutrals 131 in the same grid format as the GUMICS-4 data. The Hodges study used a Monte Carlo 132 simulation process to model the hydrogen exosphere as a function of spherics. The values 133 were given for four different solar radio flux values at 10.7 cm wavelength ($F_{10.7}$) at equinox 134 and solstice, while also being dependent upon radial distance. During each case study we 135 take the daily $F_{10.7}$ average and using the date of the observation, we interpolate between 136 the four given $F_{10.7}$ values and the temporal distance from summer solstice using day-137 of-year number. This interpolation process produces a unique neutral hydrogen grid for 138 each case study. 139

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¹⁴¹ 2.2.3. Calculating α

The alpha value is a proportional factor based on a combination of the relative abundances and the cross-section of each possible interaction between a solar wind ion and a neutral particle causing an emission line in the relevant energy range [*Cravens*, 2000]. The general equation for the calculation of this value is shown in Equation (2), where X is the element required and q is the charge state.

$$\alpha_{X^{q^+}} = \sigma E \left[\frac{X^{q^+}}{O} \right] \left[\frac{O}{H} \right]$$
(2)

In the case of calculating the oxygen emission lines we need to know the emission line energy, cross section of the interaction, abundance of the relevant charge state and the ratio of oxygen to hydrogen (O/H) in the solar wind. We use two hour time resolution,

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¹⁵¹ O/H ratio and oxygen charge state abundance data from the ACE spacecraft, timeshifted ¹⁵² to the bow shock in the same way as the OMNI data. If no solar wind composition data ¹⁵³ is available we use the values in *Schwadron and Cravens* [2000], which is discussed further ¹⁵⁴ in Section 4.2.

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¹⁵⁶ The cross section value and energy for each transition of O^{7+} (seven transitions) and ¹⁵⁷ O^{8+} (five transitions) with neutral hydrogen are based on experimental data taken from ¹⁵⁸ *Bodewits* [2007]. The cross section value for each transition is interpolated based on the ¹⁵⁹ input ion speed, from the five values given (200, 400, 600, 800, and 1000 kms⁻¹). The ¹⁶⁰ individual alpha values for each transition are then summed to produce a combined alpha ¹⁶¹ value for all relevant oxygen transitions.

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For comparison to empirical methods, the α value for the model timeframe shown in Figure 1 is 7.6×10^{-16} eV cm². This has been calculated based on the input solar wind velocity of 438 km/s, an $\frac{O}{H}$ ratio of 1.1×10^{-3} , an O⁷⁺ abundance of 0.28, and an O⁸⁺ abundance of 0.05. This value compares favourably with empirical α values of 6×10^{-16} eV cm² [*Cravens et al.*, 2001; *Robertson and Cravens*, 2003].

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¹⁶⁹ 2.2.4. Combination of the data

We now have all the requirements to produce an X-ray emissivity cube. The output of the GUMICS-4 simulation is combined with both the neutral hydrogen number density and the alpha value as shown in Equation 1. Example slices through the data grid for each of the components which are combined to form the X-ray emissivity grid are given

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¹⁷⁴ in Figure 1. Each panel shows an example 2D slice through the 3D datacube in the ¹⁷⁵ ecliptic (x-y) plane at z = 0. Panels a) to c) of Figure 1 show GUMICS-4 data output ¹⁷⁶ of the solar wind proton number density, speed and temperature respectively. Panel d) ¹⁷⁷ shows a neutral hydrogen data slice from the Hodges model. Panel e) shows the result of ¹⁷⁸ combining the model output, neutral hydrogen data and cross section values together to ¹⁷⁹ create the model X-ray emissivity.

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¹⁸¹ 2.2.5. Applying a mask

As a one fluid simulation, the GUMICS-4 MHD code does not identify the difference 182 between solar wind plasma and plasma of terrestrial origin. As a consequence we can 183 observe high terrestrial plasma densities near the Earth which in turn produce unphysical 184 X-ray emissivity. The terrestrial plasma does not contain the same ratio of highly ionized 185 oxygen species and hence cannot produce the same level of charge exchange emission. We 186 can clearly see this effect by comparing panels f) and g) of Figure 1 which are slices of panel 187 e). In panel e) we present the x-y plane of X-ray emissivity which shows some emission 188 enhancement very close to the Earth. When we examine the y-z plane with a cut taken 189 at $x = 3.9 \text{ R}_E$, in panel f), we see the extent of the terrestrial plasma. Panel g) shows a 190 cut at $x = 9 R_E$ where the emission is not affected by the terrestrial plasma. The Earth 191 size and position is also included in panels e), f) and g) for comparison. We assume the 192 boundary between the terrestrial and solar wind plasmas is at the magnetopause *Spreiter* 193 et al., 1966]. The magnetopause model given in Shue et al. [1998] defines this boundary, 194 with all proton densities (panel a) within this region set to zero. The relative merits of 195 the empirical and MHD based magnetopause are discussed in Section 4.1. 196

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2.3. Calculating an estimated instrument view

¹⁹⁷ We now have a three dimensional X-ray emissivity product in an irregular grid. To ¹⁹⁸ simulate what XMM-Newton would see we integrate along the viewing path from the ¹⁹⁹ satellite location. To determine the amount of X-ray emission directed along the line of ²⁰⁰ sight we integrate along the look vector, $\int P_X dS$, from Equation (1).

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At every 0.5 R_E step distance through the data cube from the satellite location we take 202 an interpolated emissivity value. The nearest neighbor emissivity data points within a 0.5 203 R_E radial distance are taken and averaged, with each neighbor weighting dependent upon 204 the distance from the required point. This interpolated emissivity value is multiplied by 205 the step distance and totaled to create the integral column flux. While this integral energy 206 collection value can be used for comparison, as a final step we pass both the energy and 207 appropriate spectrum of the oxygen transitions through the EPIC instrument response 208 matrix to provide a counts per second (c/s) value in the 0.5 to 0.7 keV band. The start 209 and end times of each EPIC timestep (at 1000s resolution) can then be determined and 210 an appropriate average count rate for that specific time period returned. Shorter step 211 distances were also trialed, resulting in negligible flux differences due to the weighted 212 averaging method. 213

3. Results

An initial investigation of the 30 case studies showed that the EPIC camera suffered from sparse data in six cases, which were removed from the study. Of the remaining 24 cases another five had XMM-Newton at a negative x value, i.e. antisunward, with an instrument view direction that did not intersect our datacube and these cases were also

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removed, leaving 19 case studies with data. Each case was assigned an identifying code,
comprising the year and number of the case within that year in date order (e.g. YY-C).
These identifiers have been included in Table 1.

3.1. Background removal

Processing of the raw EPIC data to produce the lightcurves used in this study is described in detail in *Carter and Sembay* [2008]. This includes the methodology for identifying and removing astrophysical point sources from the data and cleaning the data of soft-proton flares which can produce a strongly variable diffuse background.

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The residual diffuse signal is dominated by the variable foreground SWCX component and background components which are non-variable on the timescale of individual observations. This background is a combination of an X-ray component and the residual particle background in the EPIC detectors. The background X-ray component is a combination of the astrophysical X-ray background arising from emission from our Galaxy and unresolved point sources (extragalactic active galactic nuclei), and from SWCX in the wider heliosphere.

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The particle background in each observation can be estimated by a well establised procedure [*Carter and Read*, 2007]. We have estimated the X-ray background from the ROSAT all sky survey [*Voges et al.*, 1999]. For each look direction on the sky appropriate to the EPIC data we have used existing procedures within NASA's HEASARC toolkit to derive an estimated count rate in the EPIC instrument 0.5 to 0.7 keV energy band from the observed count rate in the ROSAT R4 band, which has an energy range of between

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0.44 and 1.01 keV. To make the conversion from one instrument to the other requires 240 the assumption of a spectral model. Formally the diffuse X-ray background spectrum is 241 well represented by a two-component thermal APEC model for the Galactic emission and 242 a power law for the unresolved power law [Kuntz and Snowden, 2008]. We have used 243 the spectral parameters from a deep analysis of case 01-3 previously studied by *Carter* 244 et al. [2010] modified by the appropriate absorption in the light-of-sight which is provided 245 by the HEASARC toolkit and derived from the Leiden/Argentine/Bohn (LAB) neutral 246 hydrogen survey [Kalberla et al., 2005]. Technically the spectral parameters will vary 247 according to sky position, however, the ROSAT to EPIC conversion in these bands is not 248 very sensitive to plausible variations in the parameters and the resultant uncertainty is 249 comparable to the uncertainty due to the inter-calibration between the instruments. 250

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The total estimated background for each observation is listed in Table 1. In comparison with the median observed count rate, also listed in Table 1, we can see that the background (i.e. non local SWCX components) represents between $\sim 10-40\%$ of the observed 0.5 to 0.7 keV signal in these cases.

3.2. Observation to model comparison

For each case study we produce a full set of plots including the GUMICS-4 integral energy and estimated count rate output, the solar wind conditions, the EPIC lightcurve, and satellite positional information. These plots allow us to check for errors and notice patterns in large count rate differences. An example of this type of plot is shown for case 01-1 in Figure 2. The left hand panels show; the GUMICS-4 integral energy output (a), the GUMICS-4 estimated count rate (b), the velocity and number density

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of solar wind protons (c), B_z and dynamic pressure (d), the oxygen to hydrogen ratio (e) and the oxygen state abundances (f). The right panels show; the observational data (g), a comparison between GUMICS-4 and observations before background removal (h), a comparison between GUMICS-4 and observations after background removal (i), a normalized comparison (j), the radial distance of the satellite and magnetopause (k) and the final smaller panels show the position, orbit path and look direction for the case.

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The 01-1 case is of interest as it covers a long time period (26.5 hours), shows a wide 269 range of features, and was previously examined in detail by *Snowden et al.* [2004]. We see 270 good agreement between the background removed observations and the GUMICS-4 count 271 rates (panel i) from $\sim 15:00$ onwards, including a gradual decline in magnitude starting 272 around 22:00. The start of the case study suffers from an integral emissivity which is 273 several orders of magnitude in error (panel b). This is discussed further in Section 4.1 274 but results from the mask not accurately removing all the plasma of terrestrial origin. 275 Panel f) also shows a large variation of O^{7+} abundances, ranging from 10% to almost 276 50%, which is discussed in Section 4.2. 277

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The GUMICS-4 count rate estimation comparison to the background reduced EPIC observations, i.e. panel i), for all 19 cases are shown in Figures 3 and 4, with the respective identification number from Table 1. To provide an initial comparison between the cases we determine the median count rate of both the modeled and observated lightcurve and take a ratio of the two. The magnitude ratios for each case varied between 0.11 and 20.9 with a median value of 1.65. This magnitude difference average is reasonable for

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²⁸⁵ comparison although it is highly variable within cases, as observed in Figures 3 and 4.
²⁸⁶ The correlation between the two lightcurves was also calculated for each case, the average
²⁸⁷ for all cases was 0.07 with a standard deviation of 0.52. We discuss the importance and
²⁸⁸ large variance of these values in Section 4. The correlation, based on a zero time lag cross
²⁸⁹ correlation and normalized lightcurves, rather than covariance is used due to the large
²⁹⁰ magnitude differences indicated by the magnitude ratio limits.

4. Discussion

The average magnitude ratio between modeled and observed count rates of 1.65 291 indicates the model count rates are comparable to the observations although, as previously 292 mentioned, this comes with a large variability. We can compare this ratio to the empirical 293 study of *Carter et al.* [2011] who found less than a factor of ~ 2 in magnitude difference 294 for 50% of their cases. In our study we find only 6 of 19 cases (32%) within a factor of 295 two greater or smaller (i.e., a ratio between 0.5 and 2). This difference suggests that the 296 modeled process does a poorer job of magnitude modeling than the empirical study. The 297 correlation values are of concern with a mean value close to zero, due to 8 of the 19 cases 298 (42%) returning a negative correlation. These correlations can have high values and the 299 average absolute correlation value is returned as 0.44. In an attempt to determine why 300 the simulation of the X-ray emission is not reproducing the observations accurately we 301 investigate each of the model components, as set out in Section 2.2. 302

4.1. A re-examination of the method

From Equation (1), there are four important possible sources of error in our modeled data; the MHD model, the neutral hydrogen model, the mask to remove the cold terrestrial

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The GUMICS-4 model code has been verified in a one year study [Gordeev et al., 2013] 307 and used in a range of other studies [e.g., Hubert et al., 2006; Palmroth et al., 2013]. The 308 requirements for the magnetospheric plasma simulation are well within the boundaries 309 set by GUMICS-4 of $\pm 64 \, R_E$ in y and z and up to 32 R_E in x. The main limitations 310 of the model, as described in Janhunen et al. [2012], are magnetotail reconnection and 311 near Earth plasma modeling ($<3.7 R_E$). The first limitation is not relevant as we only 312 generate X-ray emission data at x > 0 and the second limitation is taken care of by use 313 of a magnetopause position mask. It is also important to note that by its fluid nature, 314 MHD models have difficulty accurately simulating the physics in regions where details of 315 the plasma distribution function are important, such as areas where kinetic effects are 316 dominant. As we are focussing on the magnetosheath emission this is less of an issue than 317 if we were to be looking at the cusp regions. 318

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The Hodges neutral hydrogen model has been used in this study. A comparison of other 320 neutral hydrogen models was performed for equinox and solstice at high and low $F_{10.7}$ 321 values, included as supplementary material to this manuscript. The first compared model 322 was the Bonn model [Nass et al., 2006] using the coefficients from the TWINS-1 LAD data 323 [Bailey and Gruntman, 2011]. We also compared the Østqaard et al. [2003] IMAGE model; 324 while only designed to be used on the nightside, the returned values are comparable to 325 the Hodges model. The last comparison was a simple r^{-3} model with a 25 cm⁻³ number 326 density at a distance of 10 R_E [Cravens et al., 2001]. The results of each comparison show 327

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very minor differences in shape and magnitude, certainly not enough for the Hodges model to be the cause of the variations between the modeled and observed lightcurves. It should also be noted that when comparing SWCX through different parts of the magnetosheath, *Kuntz and Snowden* [2008] demonstrate that the solar wind flux is a more important factor than the magnetosheath density along the line of sight. This indicates that small differences in the Hodges number density are unlikely to make any significant differences.

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We next investigate the mask used to remove the cold terrestrial plasma. The Shue model 335 is a commonly used magnetopause positional model [e.g. Liemohn et al., 1999; Dimmock 336 et al., 2015] providing a subsolar distance and flaring value based on solar wind conditions. 337 The position of the magnetopause has been extensively tested with our model output. In 338 terms of subsolar stand off distance, the position appears reasonable most of the time 339 but as the model has no historical knowledge of the conditions it can change position 340 rapidly while the plasma simulation suggests a slower movement. This swift movement 341 results in the mask occasionally being placed within the plasmasphere as described by 342 the GUMICS-4 model, allowing the dense terrestrial plasma to be included in the X-ray 343 emission grid increasing the integral line emission by several orders of magnitude as seen 344 in the modeled emission in Figure 2a). It is apparent these large magnitude increases 345 are due to poor masking by looking at the normalized data of case 01-1, panel j) of 346 Figure 2. In this normalisation panel we have included emission along the x-axis without 347 any masking in red, by providing no mask we can determine whether large increases are 348 due to higher emission or errors in mask position. At 12:00UT in panel j) we see a very 349 large increase in integral magnitude, yet there is only a small increase in the non-masked 350

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subsolar emissivity. At this time B_z turns negative which will instantly move the Shue 351 mask position Earthward, while the MHD model will take time for this change to have 352 an effect. Gordeev et al. [2013] generally found good agreement between the empirical 353 Shue magnetopause and the fluopause [Palmroth et al., 2003] defined from GUMICS-4 354 simulations. The greatest differences were found in strong southward B_z conditions near 355 the subsolar point, where the simulated magnetopause position can be up to 15-20% more 356 distant than the Shue model. This masking issue is also discussed more fully in Kuntz 357 et al. [2015] who use a closed field line model to place the mask on their BATS-R-US 358 MHD model [Powell et al., 1999]. The closed field line approach was not used in this 359 study as the field model will respond in a similar instantaneous movement to the Shue 360 magnetopause model, resulting in similar errors. 361

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An MHD model based magnetopause has been trialed for our case studies, constructed 363 by applying a gaussian fit to the proton number density along the sub-solar line. The 364 magnetopause can then be taken as a full width half maximum distance from the central 365 location, an example is shown in panel k) of Figure 2 as the black dashed line. The 366 positional difference between the Shue and proton defined boundaries is small but the 367 proton boundary is much smoother. This model defined magnetopause produces excellent 368 subsolar distances as defined, but with no angular data the magnetospheric flanks are 369 poorly determined. During the testing process we also attempted a region threshold 370 detection method, which failed regularly due to the low intensity of the flanks compared 371 to the nose. As it is clear where the Shue method differs from the MHD model (by the 372 dramatic increase in integral emission), it is simple to remove these times by applying a 373

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This leaves only the alpha value as the main source of variation error. While the cross sectional data for all possible solar wind ions in the 0.5 - 0.7 keV range is limited, it is assumed that O^{7+} and O^{8+} are the major contributors and other ion species line spectra in this range will be negligible. Hence, we are left with the upstream data inputs on the oxygen charge state abundance and total oxygen number density. These values are highly variable over each case and so we investigate whether the variance in oxygen data from ACE is responsible for the primary variation in the simulated X-ray emission.

4.2. Oxygen composition data

Previously utilised empirical models have been run using constant values for the oxygen 383 to hydrogen ratio and the charge state abundances. Whilst these values have been used as 384 a back up for missing compositional data bins during the analysis process, the variability 385 from the ACE data to the constant values has been quite high. This in turn could be a 386 source of error either in the observed oxygen data or for models using the constant values. 387 As part of this study we have included not only the nineteen cases with data analysed in 388 the results section, but also the five cases where the XMM-Newton pointing direction did 389 not intersect the datacube. These extra cases are labelled in Table 1. 390

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³⁹² 4.2.1. Oxygen to hydrogen ratio

The model constant values of the oxygen to hydrogen ratio (O/H) are 6.45×10^{-4} for fast solar wind and 5.62×10^{-4} for slow solar wind [Schwadron and Cravens, 2000]. Investigating the data values given by ACE, suitably time delayed to the bow shock, we

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³⁹⁶ note some wide variation from these constant values. Across all 24 cases the median and ³⁹⁷ mean O/H ratios are 3.11×10^{-4} and 3.94×10^{-4} respectively with a standard deviation ³⁹⁸ of 3.01×10^{-4} . While there is likely to be a reasonable amount of error in the ACE data ³⁹⁹ values due to limited instrument sensitivity, viewing angle and resolution, this should still ⁴⁰⁰ produce an average value close to the Schwadron and Craven (hereafter referred to as ⁴⁰¹ S&C) constant values if both are representative.

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Panel a) of Figure 5 shows the O/H ratio across all 24 case studies in date order, with 403 each data point taken at a 300s resolution. The solid orange background shows the extent 404 of the mean value for each case ± 1 standard deviation. The solid blue line within each 405 region shows the mean value, while the data are shown in black. The S&C values of the 406 O/H ratio are indicated by the dashed red and blue lines for fast and slow solar wind 407 respectively. This plot is complemented by a histogram of the ratio distribution in panel 408 b) with a bin size of 5×10^{-5} . This histogram shows a skewed normal distribution, with 409 the S&C constant values intersecting at a ratio greater than the FWHM value. 410

411

⁴¹² When we compare the O/H ratio to solar wind speed, using a 500 km/s cutoff between ⁴¹³ fast and slow solar wind, the fast solar wind shows a correlation between speed and ratio. ⁴¹⁴ We also observe that a comparison of the O/H ratio to the solar wind proton density ⁴¹⁵ shows a correlation, indicating that the dynamic pressure should provide a correlation too ⁴¹⁶ (as it is based on speed and density). While the speed and density plots are not included ⁴¹⁷ for space, we have plotted the O/H ratio against the solar wind dynamic pressure in panel ⁴¹⁸ c) of Figure 5 with the slow solar wind data points in black (dashed red fit line) and the

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fast solar wind ratio values in blue (solid red fit line). We observe that as expected, the fast solar wind correlates very well ($r^2 = 0.78$), producing the power law fit shown below.

$$\frac{O}{H} = 6.42 \times 10^{-4} P_{dyn}^{-3.19} \tag{3}$$

422

421

The slow wind fit correlates poorly ($r^2 = 0.21$) which is an expected result from the lack of correlation with both speed and density. The dynamic pressure relation could simply be symptomatic of the ACE measurements increasing in signal to noise ratio as the total solar wind content increases, producing more accurate results. It should be noted that a constant ratio value defined by the median of the slow wind data ($\sim 3.17 \times 10^{-4}$) is more appropriate in these cases than using the S&C value of 5.62×10^{-4} .

429

430 4.2.2. Oxygen charge state ratios

The other data observations required in the α value determination are the O⁷⁺ and 431 O^{8+} abundances as a fraction of the total solar wind oxygen. The values taken from 432 Table 1 of Schwadron and Cravens [2000] give abundances of 0.2 and 0.07 for O^{7+} and 433 O^{8+} respectively for the solar wind. These slow wind values are used as a replacement 434 for missing observational data for all cases. The S&C abundance values for fast wind 435 are 0.03 and 0.00 for O^{7+} and O^{8+} , indicating that only 3% of the oxygen is available 436 to produce SWCX in the 0.5 to 0.7 energy range. Using these values are likely to result 437 in undetectable count rates, which from Figures 3 and 4, is clearly not the case and so 438 the slow wind abundances are used for fast wind cases as well. Figure 5 shows the mean 439 abundance taken from ACE of O^{7+} (panel d) and O^{8+} (panel e) for each of the 24 cases 440 with the expected value shown as the red dashed line. As the abundance values are given 441

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on a 2 hour resolution most cases have fewer than 5 measurements and so a standard 442 deviation is not appropriate for visualising the variance of the charge states. The error 443 bars on the plots in panels d) and e) show the maximum and minimum values in each case. 444 We note that looking at panel d), 14 of the 24 O^{7+} cases (58%) have error bars that do 445 not cross the expected value at all. The O⁸⁺ abundance ranges show a similar result with 446 13 of 24 cases (54%) where the error bars do not cross the equivalent expected value. The 447 mean and median values for all O^{7+} cases are 0.28 and 0.31, while the equivalent averages 448 for O^{8+} are 0.05 and 0.03. The mean values suggest the S&C constant abundance value 449 is acceptable for both charge states, however, this does not take into account the high 450 variability. The final panel (panel f) of Figure 5 shows the O^{7+} to O^{8+} abundances, with 451 the red dashed lines showing the appropriate expected values. The correlation between 452 O^{7+} and O^{8+} abundance is to be expected and we can fit a power law to the data (shown 453 in blue), given by $O^{7+} = 0.78 O^{8+0.32}$. 454

455

It should be noted that during our analysis we noticed that in certain cases the O^{8+} 456 abundance value from ACE reached exceptionally high values. Therefore one of the 457 conditions put in place during our analysis was that the O^{8+} abundance was not allowed 458 to exceed 0.2, any values which did were set to the Schwadron and Cravens [2000] value 459 of 0.07. This limit was an arbitrary value based on the expected O^{7+} abundance and was 460 only enforced due to a few exceptionally high abundances causing non-physical variances 461 in the GUMICS-4 simulated count rate. Three cases required this adjustment to one of 462 the O^{8+} data points; 02-3, 03-4, and 03-6. The relation between O^{7+} and O^{8+} abundances 463 in panel f) of Figure 5 suggests the O^{8+} abundance at ~0.15 may also be artifically high. 464

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The same is true for the O^{7+} abundance at ~0.52, without a reference for the range of values that this abundance can take we did not limit the O^{7+} value in this study.

5. Reanalysis with a constant O/H ratio

5.1. Removing the oxygen variation

We have observed from the rapid changes in oxygen composition and number density, 467 that the oxygen variances observed in each case are high. To attempt to determine if 468 the oxygen variance is causing strong model emission variances we have reanalysed two 469 case studies with a range of O/H and charge state abundance values. The important 470 difference is that we do not allow the oxygen values to vary over the cases. The two 471 cases (00-2 and 01-3) were chosen because of their difference from the modal oxygen value 472 in Figure 5. Case 01-3 is also the observation used in *Carter et al.* [2010] for observing 473 SWCX enhancement during a coronal mass ejection interaction with the magnetosheath. 474 Figure 6 shows the two cases with 00-2 in the left panels and 01-3 in the right panels. The 475 top row shows the original model result using ACE oxygen composition data, the blue line 476 shows the model counts and the black line is the observational data points included with 477 the appropriate errorbars. The second row of Figure 6 shows the Schwadron and Cravens 478 [2000] O/H ratio of $\frac{1}{1780}$ for slow solar wind and O⁷⁺ and O⁸⁺ abundances of 0.2 and 0.07 479 applied respectively. The third row of Figure 6 shows the results from using the modal 480 O/H ratio from Figure 5 of 2×10^{-4} and using the case mean O⁷⁺ and O⁸⁺ abundances. 481 The final row of Figure 6 shows the results from using the mean O/H ratio, O^{7+} , and 482 O^{8+} abundances from each case. These mean values for case 00-2 are 7.26×10^{-4} for the 483 O/H ratio, 0.19 for the O^{7+} abundance and 0.027 for the O^{8+} abundance. The equivalent 484 values for case 01-3 are 5.03×10^{-5} for the O/H ratio, 0.31 for the O⁷⁺ abundance and 485

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Figure 6 clearly shows that in both cases setting the O/H ratio to a constant results 488 in a simulated lightcurve variance that is a lot closer to that of the observed variance. 489 The magnitude of the ratio can be seen to directly affect the magnitude of the output 490 X-ray emission. In terms of matching the magnitudes as closely as possible, the modal 491 O/H ratio from Figure 5 provides the closest match for both examples in Figure 6. We 492 therefore recalculate all our simulated X-ray emission lightcurves using a constant O/H 493 ratio of 2×10^{-4} and the mean O^{7+} and O^{8+} abundances for each case. Each case 494 comparison is shown once again in Figures 7 and 8, which can be directly compared to 495 Figures 3 and 4. 496

5.2. Accuracy of the modeled to observed magnitudes

⁴⁹⁷ A comparison of the cases with a fixed O/H ratio and those using ACE in Figures 3, ⁴⁹⁸ 4, 7 and 8 allows an initial quality check by eye. Of the 19 cases, 11 show visible ⁴⁹⁹ improvement (58%), 5 show little to no improvement (26%), and only 3 cases show a ⁵⁰⁰ decline in both magnitude and variance matching (16%). This basic check confirms that ⁵⁰¹ we should continue the analysis with these new simulations.

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Figure 9 shows the comparison of these newly calculated model count rates to the background removed EPIC observations. The top panel shows both the mean and median magnitude ratio between the modeled and observed counts for each case. Taking the median ratios, the minimum value is 0.38, the maximum is 12.45 and the median value is 2.23. This range shows that while the median magnitude is slightly higher in ratio than

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the ACE varying modeled count rates, the range of the spread is much smaller. This 508 can be seen by the fact that 8 of the 19 case averages (42%) now sit within a factor of 509 2 higher or lower of the observation magnitude average, two cases greater than the ACE 510 O/H varying results (Section 3.2). The second panel of Figure 9 shows the correlation 511 value of the modeled and observed count rates. In comparison to the ACE varying data, 512 the median correlation is now 0.35 (compared to 0.07) with a standard deviation of 0.48513 (compared to 0.52) and 5 of the cases show negative correlation. This indicates that by 514 removing the oxygen variation we obtain much better correlations between the model and 515 observations. The median of the absolute value of correlation is 0.57 (compared to 0.44), 516 indicating that whether the case is positively or negatively correlated the variances are 517 more closely related with the O/H ratio kept constant. 518

519

The lower panel of Figure 9 shows a scatter plot of each observed count rate bin against 520 the respective modeled count rate for all cases. The scatter plot is accompanied by 521 histograms of each count rate distribution. The solid black line indicates an exact count 522 rate match between observation and modeled count rates and, as expected by the case 523 average magnitude ratio of 2.23, most of the data points sit above this line. This is 524 illustrated further by the red dashed lines which indicate the modal count rate bins, the 525 EPIC modal value of 0.087 counts is approximately half the modal GUMICS-4 count 526 rate of 0.199. This approximate factor of two is duplicated in the median of all data 527 points (blue dashed line) where the EPIC value is 0.091 compared to the GUMICS-4 528 median value of 0.218. The actual factor of 2.4 is slightly different from the case average 529 value of 2.23 due to the fact that each observation ranges in length from 3 hours to 26.5 530

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⁵³¹ hours. It should be noted that the histogram of varying O/H modeled count rates (not ⁵³² shown) resulted in a bi-modal distribution at 0.16 and 0.63 counts per second which is ⁵³³ not repeated when the O/H ratio is kept constant.

5.3. Comparing SWCX quiet and enhanced times

As well as looking at the correlation value we can also compare the model and observed 534 count rates to ensure that both are seeing more generalised X-ray emission enhancement 535 at the same time. We determine the periods of enhancement during each case from the 536 observed count rate lightcurve, given in *Carter et al.* [2011]. Each case shows a definitive 537 period of enhancement which can be either from the start of the observation, near the 538 end of the observation or sometime between the start and end. By determining these 539 enhancement cut off times we separate out the observed and model count rates for each 540 case into quiet and enhanced categories. Taking the mean count rate of both the quiet 541 and enhanced periods, we can create both a ratio and difference value between the two 542 for each case. 543

544

Figure 10 shows the values for the ratio between enhanced to quiet count rate. The top 545 panel shows the cases in data order with each symbol representing; the EPIC observed 546 ratio (green circle), the modeled ratio with an ACE varying O/H value (black star), and 547 the modeled ratio with a constant O/H value (red plus). Placing all the case values in date 548 order shows there are no temporal trends such as a decrease in accuracy with solar cycle or 549 instrument degradation. The dashed line shows the 1:1 ratio with any points falling below 550 the line indicating that the enhanced time is producing less flux. By definition, the EPIC 551 observations all fall above the ratio line with a mean increase of 48% and median increase 552

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of 22% in c/s during SWCX enhancement times. The O/H varying cases have four cases 553 where the ratio is less than 1, indicating that the SWCX enhanced period is returning less 554 X-ray emission. Whereas, for the constant O/H there are only two cases where this occurs. 555 The mean and median count rate increases for the O/H varying model are 370% and 556 53% respectively. The equivalent values for the constant O/H model are 116% and 96%557 respectively. While the varying O/H data provides a median increase between quiet and 558 enhanced times similar to that seen in the observed data, the extremely high mean value 559 indicates this is subject to high variation. The constant O/H ratio enhancement again 560 shows a factor of two in both the mean and median enhancement rates. We investigate 561 this further by plotting out each modeled enhancement ratio against the observed values 562 in the lower two panels of Figure 10. The left panel shows the ACE varying enhancement 563 ratio and the right panel shows the constant O/H enhancement ratio values, to be able 564 to show both data sets on the same scale we have plotted these on a $\log x$ axis. The solid 565 red line indicates the y=x line for ease of comparison. The variability of the results can 566 once again be seen in the ACE varying model data although around the ratio of 1.5 the 567 observations match up to the model extremely well. The constant O/H enhanced ratio 568 values show a tighter spread but a reduced accuracy in the cases which matched well in 569 the varying O/H plot. 570

571

The ratio between enhanced and quiet times will be very sensitive to the quiet time magnitudes, which in turn will be heavily influenced by the calculated background values. As a complement to the ratio calculation we have also determined the magnitude difference between enhanced and quiet times for each case, shown in Figure 11. The top panel

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shows the difference values in time order, again showing no temporal pattern between 576 observations and model results. The mean and median enhancements are 0.08 and 0.06 577 counts per second for the observed differences, 0.05 and 0.04 for the ACE varying model, 578 and 0.15 and 0.09 for the constant O/H model. The lower panels of Figure 11 show the 579 scatter plot between observed and model differences, the solid red line in each plot shows 580 the line of unity. The lower left plot also indicates the position of an outlying point at a 581 model difference value of -0.63 c/s, this has been shown in blue. The ACE varying data 582 shows a similar result to Figure 10 with a few cases correlating very well to the observed 583 differences but the spread is wider than the constant O/H model data. The data from 584 both the difference and ratio between enhanced and quiet times agrees, in some cases the 585 ACE varying data does an excellent job while setting the O/H ratio to constant produces 586 a more reliable result but reduces accuracy. 587

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The case of April 17 2002 (02-2) has no enhanced to quiet ratio for either O/H value as the enhancement occurs in the final two bins of the observation and neither simulation returns counts for this period.

5.4. Positional accuracy

⁵⁹² As a final piece of analysis we have also displayed the spatial position of the model data ⁵⁹³ using a constant O/H ratio in Figure 12. The left panel shows the data in a cylindrical ⁵⁹⁴ coordinate system (x-r) with the r axis signed by whether the y value is positive or ⁵⁹⁵ negative. This view gives us positional values projected onto a 2D plane with a 0.5 R_E by ⁵⁹⁶ 1 R_E resolution. We have binned all the data points and taken the average integral count ⁵⁹⁷ rate for each bin, with our limited number of case studies this leaves a large proportion

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of the grid without any data but does show that the higher modeled count rates occur 598 when the satellite is looking in the positive y direction (dusk). The top right panel of 599 Figure 12 shows the data binned in the y-z plane, with no dependence upon the x value. 600 We can again observe the asymmetry in y but the highest count rates occur at the z values 601 closest to zero, as these values are likely to be closest to the nose of the magnetosheath it 602 could simply be a proximity relation to the highest emission rates. To determine whether 603 distance from the magnetopause is significant we plot each model count rate against the 604 radial distance from the Shue magnetopause during the specific data point conditions. 605 This scatter plot is shown in the middle right panel of Figure 12, with the data points 606 split by y position. The positive y values are shown by black + signs and the negative y607 values are shown by blue * symbols. When looking at all the data points combined we 608 can see that the count rate increases with distance from the magnetopause. This result 609 is initially counterintuitive as we would expect the count rate to be higher the deeper in 610 the magnetosheath the satellite is. What must be considered is the pointing direction 611 and case selection bias. A case where the satellite is far from the magnetopause would 612 only have shown initial significant SWCX if the pointing direction intersected a significant 613 fraction of the magnetosheath. As the satellite comes closer to the Earth the integral path 614 through the data grid includes fewer bins. If we took a sample of spacecraft positions with 615 the spacecraft pointing in random directions then the opposite relation should be true. 616 This magnitude plot shows, in a similar manner to the binned grid plots, that the count 617 rates when y is positive are generally higher. The final plot of Figure 12, in the lower 618 right panel, shows average distance from the magnetopause with correlation between the 619 observed and modeled lightcurves. These data points are again split by whether y is 620

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positive or negative. There appears to be no general pattern between lightcurve variance and magnetopause distance, although the highest correlations occur in the negative *y* value (dawn) data values. This asymmetry was also mentioned in *Carter et al.* [2011], where they found that the empirical model fitted better in the dawnside. This dawndusk asymmetry could be related to the known asymmetries in either the magnetosheath plasma conditions [e.g. *Walsh et al.*, 2012] or magnetopause position [e.g. *Dmitriev et al.*, 2004], indicating that this asymmetry needs to be considered during the modeling process.

6. Conclusions

In this study we have taken the data from 19 case studies using the EPIC-MOS 629 instruments on XMM-Newton to examine the accuracy of MHD modeling when describing 630 solar wind charge exchange from the Earth's magnetosheath. We found that a large 631 amount of variation in the modeled lightcurve was caused by variations in the oxygen 632 to hydrogen ratio and abundances of oxygen charge states. In a large number of these 633 cases setting the oxygen to hydrogen ratio to a constant improved the variance matching. 634 These modeled data values with a constant O/H ratio and mean charge state abundances 635 were then compared to the observed lightcurves, providing an average correlation value 636 of 0.35. This correlation has been reduced by the fact that five of the nineteen cases are 637 anti-correlated. The average magnitude ratio is a factor of 2.4 when averaging across all 638 data points, giving 42% of the cases having an average magnitude within a factor of two 639 of the observed data values, a slight decrease on the empirical method used in *Carter* 640 et al. [2011]. The highest modeled count rates occur when the satellite is in the positive 641 GSE y, with the highest correlations arising in negative y (dawn). 642

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It is clear from Sections 4.2 and 5 that the oxygen data inputs to the MHD model include 644 substantial errors. The O/H variances cause large changes in the modeled lightcurves 645 which are simply not seen in the observed lightcurves for a significant number of cases. The 646 longer (temporally) the case is, the more likely that a constant O/H ratio is inappropriate, 647 yet accurate data is needed. The same applies to the oxygen charge state abundances, the 648 two hour resolution of this data is low for modeling that runs at a four second calculation 649 resolution and a five minute grid output. The absolute abundance values themselves are 650 also an issue, it is unknown what the upper and lower limits of O^{7+} and O^{8+} should be. 651 We observed in Figure 5 that the O^{7+} abundance can take a wide range of values, up 652 to 52% which is likely unphysical. It is certain that the values given in Schwadron and 653 Cravens [2000], while of the right order of magnitude, are of limited use for this particular 654 modeling, especially as they describe almost no highly charged states in the fast wind. 655 To improve on model accuracy we either require more accurate and numerous solar wind 656 oxygen observations closer to the Earth, or an accurate proxy such as an extension of 657 the proton entropy correlation work by Pagel et al. [2004] to include the O^{8+}/O^{7+} ratio. 658 Using a constant value for the O/H ratio of 2×10^{-4} , and mean oxygen charge states for 659 each case we have removed a large amount of this variation at the cost of a small accuracy 660 loss (e.g., Figures 10 and 11). 661

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The accuracy of the MHD modeling ranges from anti-correlated to an excellent correlation. We can link several of the errors in both magnitude and variance to the oxygen data, and the disparity of the MHD magnetopause position to the Shue model. The other data

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inputs to the MHD model behave well and we have some excellent comparisons as seen in 666 Figures 7 and 8. When comparing the MHD model to the empirical model used in *Carter* 667 et al. [2011] we can say that it performs equally well. The slight decrease of magnitude 668 matching, 42% rather than 50%, of cases within a factor of two, could easily be due to 669 the background removal. Decreasing the background removal values by 0.03 c/s actually 670 increases the magnitude comparison accuracy to 63%, hence showing the importance of 671 the background removal when we look at comparing the magnitudes. The background 672 removal does not affect the correlation or the enhanced to quiet differencing comparison 673 however. Examining the magnitude difference between quiet and enhanced periods, we 674 see very similar results between the observed values and the MHD model. The difference 675 in the dawn-dusk correlations, also seen in *Carter et al.* [2011], suggests that there could 676 be an asymmetrical process affecting the charge exchange emission magnitude, which is 677 missing from both models. 678

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Users wishing to estimate the near-Earth SWCX values are advised that using either 680 the empirical model or an MHD model with constant solar wind oxygen parameters are 681 equally likely to produce a useable value. When comparing enhanced to quiet times, i.e., 682 taking an average over a longer time period, using the variable O/H data is likely to be 683 a valid approach. For those interested in a more in depth view of what is happening in 684 terms of global SWCX around the Earth, the MHD based model with a constant oxygen 685 ratio and abundances, will produce a more accurate result, including matching short time 686 scale emissivity variation. This study also acts as a validation of the model methodology 687 for global imaging of the magnetosheath using SWCX, by providing similar emissivities 688

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to observed values. However, the relative inaccuracy of using a far upstream monitor for the solar wind conditions can affect the model results considerably. This modeling will be especially important for future missions involving wide angle X-ray imaging of the Earth's magnetosheath.

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Figure 1. a) - d) The GUMICS-4 output for a single timestep showing solar wind proton number density, bulk flow speed and temperature with the final panel showing the equivalent Hodges neutral hydrogen density. Each of these panels shows a slice through the data cube in the x-y plane at z = 0. e) The calculated X-ray emissivity in the x-y plane, with cuts taken to show the y-z plane at $x = 3.9R_E$, the magnetopause sits around a subsolar distance of $9R_E$ and the bow shock is at approximately $11R_E$.

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lightcurves, **k**) XMM position relative to the magnetopause, and the final panels show the orbital position.

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Figure 3.Cases 1-9 of the study, each panel shows the GUMCIS-4 estimated count rate in
blue and the EPIC observations in black with the combined observational and background error
bars included.bars included.
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Figure 4.Cases 10-19 of the study, each panel shows the GUMCIS-4 estimated count rate in
blue and the EPIC observations in black with the combined observational and background error
bars included.
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Figure 5. A selection of plots showing the variation in oxygen to hydrogen ratio and the oxygen charge state abundance. a) The O/H ratio for every OMNI data point used in the 24 case studies with data, b) the ratio in a histogram format. c) The slow and fast O/H ratio against solar wind dynamic pressure. d) and e) The average O^{7+} and O^{8+} charge state abundance for each case. f) The O^{7+} charge state abundance plotted against the O^{8+} abundance.

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Figure 6. A comparison of changing the oxygen to hydrogen ratio. Each panel shows the XMM-Newton observations for cases 00-2 and 01-3 (in black with errorbars) as well as the GUMICS D R A F T February 12, 2016, 2:39pm D R A F T simulation in blue. Keeping the O/H ratio constant produces a variation in the simulated light curve closer to the observed values, in comparison to the ACE varying O/H ratio in the top panels.



Figure 7. Cases 1-9 of the study using a constant O/H ratio, each panel shows the GUMCIS-4 estimated count rate in blue and the EPIC observations in black with the combined observational and background error bars included $D = R = \frac{1}{4} + \frac{1}$



Figure 8.Cases 10-19 of the study using a constant O/H ratio, each panel shows the GUMCIS-4estimated count rate in blue and the EPIC observations in black with the combined observationaland background error bars included.D R A F TFebruary 12, 2016, 2:39pmD R A F T



Figure 9. A comparison of the observed and modeled count rates for each case, using the constant modal O/H value from Figure 5. The top panel uses the mean and median magnitude for each case and takes the ratio of the modeled to the observed magnitudes, with the dashed line showing the equal magnitude line. Data points below this line show a lower modeled than observed average magnitude. The middle panel shows the correlation between modeled and observed counts. The lower panel is a scatter point of all data points, with histograms included for high the modeled and observed grant observed and observed and observed states the show the solution between modeled and blue dashed lines show the panel is a scatter point of all data points, with histograms included for both the modeled and observed states the solution between the panel is a scatter point of all data points with histograms included for both the modeled and observed with the solution between the panel is a scatter point of all data points. The panel is a scatter point of all data points with histograms included for both the modeled and observed by the panel is a scatter point of all data points. The panel is a scatter point of all data points with histograms included for both the panel and observed by the panel black dashed lines the panel black dashed line shows the y=x line.



Figure 10. The ratio between the enhanced and quiet charge exchange periods of the lightcurve. The top panel shows the ratio for the O/H varying model data (*), O/H constant model data (+) and the observed data (o). These are in date order to determine any temporal bias. The lower left panel shows a scatter plot of O/H varying model data against the observed data, with the red solid line showing the y=x line. The error bars on the observed data have been propogated from the background and observational data. The lower right panel shows the same plot but with the O/H constant data points.



Figure 11. The difference between the enhanced and quiet charge exchange periods of the lightcurve. The top panel shows the ratio for the O/H varying model data (*), O/H constant model data (+) and the observed data (o). These are in date order to determine any temporal bias. The lower left panel shows a scatter plot of O/H varying model data against the observed data, with the red solid line showing the y=x line. The error bars on the observed data have been propagated from the background and observational data. The lower right panel shows the same plot but with the O/H constant data points. D R A F T February 12, 2016, 2:39pm D R A F T



Figure 12. The distribution of GUMICS-4 count rate distribution. a) A cylindrical plot in the x-r plane with r signed by y showing the average modeled count rate in each bin, based on the position of XMM-Newton. b) The count rates binned in the y-z plane. c) A scatter plot showing the GUMICS-4 count rate values against distance from the magnetopause. d) The correlation between GUMICS-4 and observations for each case plotted against the average distance from the magnetopause.

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Table 1. List of the XMM-Newton observation cases used in this study. The mean case magnitude, pre background removal, is included as well as the calculated background value, both in c/s and as a percentage of the case magnitude. Rejected cases are due to the instrument pointing into the nightside of the Earth where we don't use the MHD model.

Case	Revolution	Obs ID	Date	Duration (hrs)	$\begin{array}{c} \text{Magnitude}^1 \\ \text{(c/s)} \end{array}$	$\begin{array}{c} \text{Background} \\ \text{(c/s)} \end{array}$	
	2000						
00-1	0114	0127921101	23 Jul	2.5	0.319	0.129 (40.4%)	
00-2	0139	0109060101	$11 { m Sep}$	14.5	0.146	0.048 (33.2%)	
	2001						
01-1	0271	0111550401	01 Jun	26.5	0.179	0.050(28.1%)	
01-2	0339	0054540501	16 Oct	6.5	0.300	0.032~(10.9%)	
01-3	0342	0085150301	21 Oct	9	0.306	0.059~(19.2%)	
	2002						
02-1	0422	0113050401	29 Mar	7.5	0.444	0.101 (22.8%)	
02-2	0431	0136000101	$17 \mathrm{Apr}$	6	0.298	0.077(25.9%)	
02-3	0494	0109120101	21 Aug	11	0.165	0.038~(23.0%)	
02-4	0529	0147540101	29 Oct	7	0.232	0.089~(38.5%)	
	2003						
03-1	0605	0146390201	29 Mar	6.5	0.215	0.077~(35.6%)	
03-2	0623	0150610101	04 May	3	0.288	0.107 (37.2%)	
03-3	0630	0143150601	18 May	5.5	0.291	0.080(27.7%)	
03-4	0657	0141980201	11 Jul	6	0.398	0.107(27.0%)	
03 - 5	0664	0150680101	26 Jul	13	0.268	0.059~(22.0%)	
03-6	0676	0049540401	19 Aug	7	0.254	0.082~(32.2%)	
03-7	0690	0149630301	$16 { m Sep}$	5.5	0.331	0.116~(35.0%)	
	2004						
04-1	0811	0202100301	14 May	7	0.228	0.079(34.6%)	
	2005						
05-1	0997	0303260501	20 May	9.5	0.164	0.037~(22.4%)	
05-2	1014	0305920601	23 Jun	7	0.267	0.105 (39.4%)	
Reje	ected cases						
	0151	0094800201	05 Oct	2000			
	0163	0100640201	29 Oct	2000	2		
	0178	0110980101	27 Nov	2000	2		
	0178	0101040301	28 Nov	2000	2		
	0209	0093552701	28 Jan	2001			
	0279	0070340501	18 Jun	2001	9		
	0505	0153752201	11 Sep	2002	2		
	0645	0150320201	17 Jun	2003	0		
	0906	0203361501	19 Nov	2004	2		
т	0982	0306700301	19 Apr	2005 $201602 \cdot 3$	89mm	ת	R. A
-	1199	0402250201	27 Jun		° r'''	D	10 11

¹ Mean case magnitude before background removal.

 2 The pointing direction is away from the datacube, providing no data. However, the case can

still be used for solar wind information.

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