Predicting geostationary 40-150 keV electron flux using ARMAX (an autoregressive moving average transfer function), RNN (a recurrent neural network), and logistic regression: a comparison of models

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Key Points:

• Regression models incorporating interaction and quadratic terms predict electron flux as well as neural network models

- The description of time series behavior by ARMAX models, while useful for hypothesis testing, is not necessary for prediction
- MLT as a predictor improves the models by describing changing flux levels and the differing influence of parameters over the diurnal period

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This is the author manuscript accepted for publication and has undergone full peer review but has not been through the copyediting, typesetting, pagination and proofreading process, which may lead to differences between this version and the Version of Record. Please cite this article as doi: 10.1029/2022SW003263.

Abstract

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We screen several algorithms for their ability to produce good predictive models of hourly 40-150 keV electron flux at geostationary orbit (data from GOES-13) using solar wind, IMF, and geomagnetic index parameters that would be available for real time forecasting. Value-predicting models developed using ARMAX (autoregressive moving average transfer function), RNN (recurrent neural network), or stepwise-reduced regression produced roughly similar results. Including magnetic local time (MLT) as a categorical variable to describe both the differing levels of flux and the differing influence of parameters improved the models (r as high as 0.814; Heidke skill score as high as 0.663), however value-predicting models did a poor job at predicting highs and lows. Diagnostic tests are introduced (cubic fit to observation-prediction relationship and Lag1 correlation) that better assess predictions of extremes than single metrics such as RMSE, MAE, or MSA. Classifier models (RNN and logistic regression) were equally able to predict flux rise above the 75th percentile (Heidke skill score as high as 0.667). Logistic regression models were improved by the addition of multiplicative interaction and quadratic terms. Only predictors from 1 or 3 hours before were necessary and a detailed description of flux time series behavior was not needed. Stepwise selection of these variables trimmed non-contributing parameters for a more parsimonious and portable logistic regression model that predicted as well as neural network-derived models. We provide a logistic regression model (LL3: LogisticLag3) based on inputs measured 3 h previous, along with optimal probability thresholds, for future predictions.

Plain Language Summary

As high levels of electrons in the radiation belts can damage satellites, accurate forecasting would be a useful tool. Electron levels can be predicted using information from the solar wind, the interplanetary magnetic field, and indices measuring disturbances in Earth's magnetic field. We compare several algorithms to produce such models: regression and neural networks that depend on predictors at one or many previous time steps. We find that dependable predictions can be made from a regression model using predictors from only a single previous time step. More sophisticated neural network techniques are not necessary if interaction and nonlinear terms are introduced to the regression.

1 Introduction

Electrons in the radiation belts can cause both internal and surface charging of spacecraft (e.g., Lam et al., 2012; Loto'aniu et al., 2015), with internal charging mainly due to >100 keV (kiloelectronVolt) electrons and surface charging to electrons below 100 keV. However, while daily averaged >100 keV electron fluxes can be reasonably well predicted because they often result from geomagnetic storms (e.g., Subbotin & Shprits, 2009; Pakhotin et al., 2014; Glauert et al., 2014; Balikhin et al., 2016; Simms et al., 2016), the same is not true of <100 keV electrons. Not only do these lower energy electrons result in the more damaging surface charging, they are also much more difficult to forecast (e.g., Koons et al., 2000; Choi et al., 2011; Matéo-Vélez et al., 2018). For LANL (Los Alamos National Laboratory) satellites, for example, it is the energy range of $\sim 10-50$ keV that is most important for surface charging (Thomsen et al., 2013; Matéo-Vélez et al., 2018). These lower energy electrons vary on time scales of minutes with their distribution depending on location in the magnetosphere, so daily/orbit averaging is not possible. Moreover, geomagnetic storms are not always predictive of keV electron enhancements, and surface charging events have been detected during even weak to moderate substorm activity (Matéo-Vélez et al., 2018; Ganushkina et al., 2021).

Electron fluxes at keV energies have been modeled with several techniques, including a first principle kinetic approach in several ring current simulations (e.g., Fok et al., 2014; Ganushkina et al., 2014; Chen et al., 2015; Jordanova et al., 2016), empirical models using different fittings (e.g., Roeder et al., 2005; Sicard-Piet et al., 2008; Ginet et al., 2013; Denton et al., 2015, 2016; Sillanpää et al., 2017), and multivariate approaches including conditional mutual information (Stepanov et al., 2021) and Nonlinear AutoRegressive Moving Average with eXogenous (NARMAX) inputs (Boynton et al., 2013, 2016, 2019). However, these empirical models may depend on only a few parameters. A wider array of input parameters could improve predictions of keV electron fluxes. Solar wind and IMF (Interplanetary Magnetic Field) parameters alone may produce reasonable predictive models, with the advantage that these would be readily available for real time forecasting.

Several studies have examined the response of geosynchronous keV electron flux to solar wind parameters, with electron enhancements associated with pressure increases (Shi et al., 2009) or higher solar wind speed (Li et al., 2005; Kellerman & Shprits, 2012; Hartley et al., 2014). A combination of solar wind speed and the IMF B_z has been found to be predictive as well (Sillanpää et al., 2017), with lesser influence from the other two IMF components and solar wind density, temperature, and pressure (e.g., Li et al., 2005; Kellerman & Shprits, 2012; Ganushkina et al., 2019). This suggests that combinations of parameters, whether multiplicative or additive, may best predict flux, reflecting multiple driving parameters (Denton et al., 2016). As keV electrons levels fluctuate on time scales of hours, better models may come from prediction parameters at a similar cadence.

Higher energy electrons (MeV; MegaelectronVolt), when daily averaged, have shown high correlations with solar wind parameters (wind speed and density either individually or in combination) (e.g., Blake et al., 1997; Paulikas & Blake, 1979; Li et al., 2001; Reeves et al., 2011; Lyatsky & Khazanov, 2008; Balikhin et al., 2011). However, the hourly response may be much lower (Simms, Engebretson, & Reeves, 2022), and the physical influence of many solar wind drivers on even MeV electron flux may not be as high as these correlations suggest. Much of the solar wind influence may not be direct but instead mediated by waves and electron injections following substorms (e.g., (Simms et al., 2018a)), and simple correlations of solar wind parameters with electrons may be inflated by common cycles and trends if these commonalities are not removed via such methods as a differencing transformation or ARMAX modelling (Simms, Engebretson, & Reeves, 2022). However, for prediction purposes, it may not be important that variables physically drive keV electron flux, nor that the correlations are only due to mutual cycles. Highly correlated proxies may be sufficient for prediction, and more practical given their real-time availability. For keV electrons, the strongest solar wind correlates are some combination of velocity, density and pressure (Ganushkina et al., 2019; Simms, Ganushkina, et al., 2022). IMF B_z , while it does not show as high a correlation as solar wind velocity, may still be a useful addition as it provides further information not present in the solar wind parameters alone. (The southward component of IMF (B_s) may appear to be a more targeted version of this parameter and therefore likely of more predictive use, but we have found that B_s does not correlate better with flux than B_z itself, at least in hourly data (Simms, Ganushkina, et al., 2022)).

Geomagnetic indices are easy to obtain measures that have often been used in prediction models. Although there may be concern that ground-based indices (measured at ground magnetometers), may not represent conditions in the magnetosphere well, they are worth testing as possible predictors that contain, at least, some information that we do not have access to otherwise. Bearing in mind that they may be proxies of pertinent physical processes that all manifest as magnetic perturbation in a single number, we can still use these for prediction purposes. However, although the AE (Auroral Electrojet) index may be a reasonable measure of substorm activity that correlates well with keV electrons (Ganushkina et al., 2021) due to its ability to indicate electron injections, it is not useful for real time predictions because it is not published immediately. If we cannot use AE, two other indices, Kp (Planetarische Kennziffer) and SymH (symmetric H-component of the ground magnetic field, or Dst (Disturbance Storm-Time), show sim-

ilarly high simple correlations with flux. Neither Kp nor SymH show as much association with flux as AE does when all 3 of these indices are included in the same analysis, but they may be a practical second choice for prediction purposes. Kp correlates well with 1-40 keV flux (e.g., Freeman, 1974; Korth et al., 1999; Thomsen et al., 2013; Denton et al., 2015, 2016). Its 3 hour cadence may make it too slow to measure quick changes in geomagnetic activity that may be associated with fast electron enhancements, but its inclusion in a prediction model may be helpful to measure the general background level of disturbance. SymH would be the obvious choice as it is reported at a 1-min cadence, but it is not currently available in real time for prediction purposes. Given this problem, Dst may be the best geomagnetic index parameter to include in a prediction model as it is available in real time and at an hourly cadence (improving over the 3 h Kp cadence). As SymH is essentially the Dst index at finer time resolution (minute vs hourly), the choice of Dst over SymH should make no difference in the prediction of hourly electron flux (Iyemori et al., 2010). It also may be useful to incorporate the solar energy flux (f10.7) even though it changes relatively slowly.

Previous work has also explored the effect of polynomial (Balikhin et al., 2011) and polynomial and multiplicative interaction terms (Simms et al., 2018b). The quadratic (square) and cubic terms of predictors can account for possible nonlinear effects that are not dealt with by log transformations, while multiplicative interaction terms describe the synergistic effects of variable pairs. Polynomial and multiplicative terms such as this will either be incorporated automatically by a neural network approach, if the algorithm finds them useful, or can be included as additional terms in ARMAX or regression models.

In this study, we explore the ability of several multivariable prediction model types to predict electron flux that have been used at various electron energies: neural networks (for example, Simms and Engebretson (2020); Koons and Gorney (1991); Ling et al. (2010); Freeman et al. (1998); Smirnov et al. (2020)); Ma et al. (2022); Katsavrias et al. (2022); Chu et al. (2021); Swiger et al. (2022)), autoregressive moving average time series transfer functions (ARMAX) (Balikhin et al., 2011; Boynton et al., 2013, 2015; Simms et al., 2018a; Simms & Engebretson, 2020), conventional regression (value-predicting) (Simms et al., 2014, 2016), and logistic regression (which classifies predictions into groups) (Simms & Engebretson, 2020; Capman et al., 2019; Neter et al., 1990).

In the present paper, we explore the capabilities of three approaches, namely, recurrent neural networks (RNN), ARMAX and conventional and logistic regression, to model hourly electron fluxes with energies of 40-150 keV as observed at geostationary GOES-13 satellite using solar wind, IMF, and geomagnetic indices as parameters. Models may be either value-predicting (RNN, ARMAX, conventional regression), or predict the probability of being over a given threshold value (RNN, logistic regression). Either ARMAX or conventional regression values output can also be categorized as above or below a threshold (although they do not predict probability). We also take the opportunity to briefly compare the power of several single-value metrics to distinguish between model prediction ability. (However, for a more comprehensive comparison see Liemohn et al. (2021).) We note that these single-value metrics are heavily weighted by mid-range values and are not well suited to assessing how well a model predicts the high electron fluxes that are of most interest. We propose several other assessment techniques, but this is not the main focus of this study which, instead, seeks to determine whether or not model predictions can be improved by various methods.

Section 2 gives a brief description of the GOES-13 MAGED data used in this study. Section 3 outlines the steps for building the models used in the study. Assessing and validation results of the three models' outputs over the GOES-13 MAGED data are presented in Section 4 including predictions above the threshold for model comparison. Section 5 is devoted to the building of probability prediction models which can give more accurate predictions than models predicting flux values. The obtained results are discussed in Section 6 and the conclusions are drawn in Section 7.

2 Data

We use hourly averaged electron fluxes (centered at midpoints of 40, 75, and 150 keV) from the geostationary GOES-13 satellite. Directional differential electron fluxes $(cm^{-2} \cdot s^{-1} \cdot sr^{-1} \cdot keV^{-1})$ from the nine collimated solid state telescopes of the MAGED instrument (e.g., Rowland and Weigel (2012)) each have a 30° full-angle conical field of view. We compute one omnidirectionally averaged flux (flight direction-integrated differential electron flux) for each of the energies using pitch angles calculated from the GOES Magnetometer 1 data following the method presented in Sillanpää et al. (2017) and Ganushkina et al. (2019). The GOES-13 MAGED data of electron fluxes and the data for the pitch angles of each telescope are available at

https://www.ncei.noaa.gov/data/goes-space-environment-monitor/access/full/

We use data covering 10 June 2013 - 6 August 2016 to build the models (the training set) and the 7 August 2016 - 12 December 2017 period for validation (the test set). There were minimal data gaps of only several hours during these time periods. These gaps were filled using linear interpolation between existing observations. This was necessary for the ARMAX models which require complete time series. Because the ARMAX models require a continuous time period for each of both the training and validation sets, cross-validation using a number of randomly selected sets out of the data is not possible. Therefore, to compare model performance on the same data, models were all built on the same training set and validated on the same withheld test set. Due to data availability, the models are built on observations from the solar cycle peak moving into the declining phase, but validation is performed on a withheld test set from further in the declining phase. This could potentially reduce the effectiveness of predictions if electron flux response to solar wind, IMF, and geomagnetic parameters were to vary over the solar cycle. While the average levels of these parameters vary over the solar cycle, we are unaware of any evidence suggesting that the flux response to a given level changes. However, given this possibility, further work should attempt validation of these models with periods during different phases of the solar cycle.

Solar wind parameters (solar wind velocity V, number density N, pressure P, the solar flux f10.7 index (SolarFlux), IMF B_z and electric field E_y , and magnetic indices (Kp and Dst) were obtained from OMNIWeb

(https://omniweb.gsfc.nasa.gov/form/dx1.html) with 1 h resolution with data timeshifted to the bow shock nose.

We take log_{10} of all variables ≥ 0 . Variables containing zero values which cannot be logged without creating missing values (i.e., Kp) were transformed by adding 1 to all values before the log transformation. B_z and E_y , as they have both positive and negative values, were not logged. A log transformation of electron flux data linearizes the relationship between predictors and response, allowing the use of techniques that assume this such as regression and neural networks (Simms, Ganushkina, et al., 2022). This transformation reduces skewness, inequality of variances among groups, and the non-normality of residual errors, all of which would make the use of linear models invalid. Examination of residual plots of the linear ARMAX and regression models (not shown) showed that this transformation fixed all these problems.

Because the dependent variable (electron flux) is log-transformed, these models will describe a nonlinear relationship between flux and all the variables: a power function relationship for those predictor variables that are also log-transformed, and an exponential function relationship for those predictor variables that are not logged. Subsequent to the log transformation, all variables were standardized by subtracting that series mean and dividing by its standard deviation. This creates unitless variables (Z-scores) for which regression coefficients (slopes) can be directly compared (Neter et al., 1990) but is also necessary for both efficient convergence and accuracy of prediction in neural networks (Alpaydin, 2014). An additional benefit is that scaling all output variables to the same

| | Mean | Std Dev |
|-----------------------------|----------|---------|
| $\log 40$ keV Flux | 4.5066 | 0.4152 |
| $\log 75$ keV Flux | 4.2019 | 0.3954 |
| $\log 150 \text{ keV Flux}$ | 3.6587 | 0.4241 |
| log B | 0.7458 | 0.186 |
| Bz | 0.0393 | 3.1674 |
| Ey | -0.0186 | 1.3692 |
| log N | 0.7906 | 0.2826 |
| $\log V$ | 2.611 | 0.0868 |
| log P | 0.2362 | 0.2691 |
| $\log (Kp+1)$ | 0.4017 | 0.1995 |
| Dst | -11.4803 | 17.4235 |
| log Solar Flux | 2.0805 | 0.0963 |

 Table 1. Means and standard deviations used to calculate Z scores.

standard deviation allows direct comparison of metrics such as the RMSE between models and output variables that might otherwise show differences in the metrics only due to different scaling. The means and standard deviations are given so that readers can backtransform to the actual flux and predictor values if desired (Table 1).

ARMAX models were developed in IBM SPSS Statistics (formerly known as the Statistical Package for the Social Sciences). RNN and regression (as well as logistic regression) models were developed in MATLAB.

3 Building Value-Predicting Models: ARMAX, RNN, and Regression

One of the more popular classes of prediction model algorithm are neural networks. As we are working with time series data, we have chosen a type specific to this type of data: an LSTM RNN model (Long Short Term Memory- Recurrent Neural Network) (Hochreiter & Schmidhuber, 1997). This type of model uses an input sequence (e.g., we use the 48 h previous of each predictor variable), with the LSTM layer "learning" the long term time dependencies between time steps. Pathways can also be "forgotten" if they are determined to contain little information, giving a more parsimonious and less overfitted model. This model type can produce either values or classification output depending on the output layer chosen. This allows us to compare output validation to either a value-output model (such as ARMAX or conventional regression) or to a probability (classification) model such as logistic regression (see below). RNN models (or any neural network) automatically test more than just the main effects of each predictor variable. The algorithm will also test multiplicative interactions between variables and polynomial terms, describing the nonlinear relationships more completely. We also attempt to refine the predictions from the RNN models by creating a different model for each magnetic local time (MLT).

ARMAX models incorporate terms to describe the time series behavior of the dependent variable (autoregressive (AR) and moving average (MA) terms), as well as exogenous predictor variables, the transfer function (represented by X) (Hyndman & Athana253

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sopoulos, 2018; Simms et al., 2019). The AR and MA terms are chosen to represent the cyclical behavior such as the daily variations in flux due to the satellite orbit. Predictor variables can be limited to the standard main effect of each parameter, or, additionally, include terms to describe the polynomial response (such as in the NARMAX models of Balikhin et al. (2010) and Boynton et al. (2011)), or synergistic action between predictors (multiplicative interaction effects), or decay terms to describe the influence from time steps in the past. The response variable can also be differenced, a transformation where each observation is subtracted from itself (e.g. $y_t - y_{t-1}$), in which case the model would be called an ARIMAX model. However, we did not find this to be a necessary transformation for this data once the time series was described with appropriate AR and MA terms. The ARMAX or ARIMAX model formulation is useful for removing cycles that can result in spurious correlations between variables and therefore avoiding erroneous conclusions about the physical driving of a system (Simms, Engebretson, & Reeves, 2022). However, the method has also been suggested as a means to better predict electron flux (Balikhin et al., 2011; Boynton et al., 2013, 2015). The output of an ARMAX model will be values, although these can be categorized if classification is desired. In the ARMAX models, we include both an influence term (from 1 h previous) and a decay term for each solar wind, IMF, and magnetospheric input variable (Hyndman & Athanasopoulos, 2018). This incorporates the continuing effect of each variable over previous hours.

Multiple regression can also be used to predict electron flux. In the simplest case, regression models can be a model of main effects. However, polynomial terms for each predictor, and the multiplicative terms between them, can also be entered to describe the variation more fully. There is also the possibility of entering predictors from many previous time steps, similar to the RNN procedure. This may lead to overfitting and an unnecessarily complicated model, but, similar to the RNN "forgetting" of inessential pathways, stepwise regression can be applied to a logistic regression model to remove predictors that do not contribute explanatory power. In this method, predictors are added or removed one by one, checking whether this improves the model at each step. The stepwise procedure is an improvement over backward elimination used previously by Camporeale et al. (2022) as it also incorporates forward selection, giving variables the opportunity to be selected at a later stage if they were eliminated prematurely. While the indiscriminate use of stepwise procedures to identify physical drivers is problematic (Whittingham et al., 2006; Smith, 2018), the same concern does not apply when developing predictive models. With a prediction model we are only concerned with the result (the prediction) and not whether the variables used to make that prediction are physically meaningful. Logistic regression, if given the same variables to work with and if reduced by stepwise regression, may find essentially the same relationships as RNN and thus be just as good at prediction. However, a regression model will be the most portable of these three model types as the coefficients can be easily printed or coded without the need for the end user to have access to the particular software the model was developed in.

Both ARMAX and RNN empirical models would appear to have an advantage over more conventional multiple regression models. RNN has the ability to incorporate predictor values from many previous time steps while with ARMAX models the time behavior of the dependent variable is modeled using AR and MA terms. This modelling of past behavior or associations would, hopefully, improve the predictions. However, it is possible that electron flux, particularly below 200 keV, is not dependent on the long term states of the magnetosphere or solar wind, or that these states are long lasting enough that correlation to just a few previous time steps holds enough information to create an accurate prediction. If that is the case, then conventional regression models should perform just as well for predictions.

We incorporate a number of solar wind, IMF, and magnetospheric variables, the only constraint being that they must be available in real time for predictions. We also, to some of the ARMAX and regression models, add a variable to identify MLT. In previous work, ARMAX models have been built for each MLT (Boynton et al., 2019). We modify this approach by providing a model for the entire time series, but with MLT as a categorical variable. In practice, this is actually a set of 23 indicator variables (0 or 1), one less than the number of hours. The coefficients of these add or subtract to the constant term of the model to describe variations in flux related to MLT. We also add multiplicative interaction terms between each of the other (continuous) variables and these indicator variables. These interaction coefficients describe how the slope or association of that continuous variable with flux changes over the 24 h of the day. The use of indicator variables essentially creates a different model for each level of the categorical variable but makes more effective use of the available information in the data.

We train each of the model types above to predict electron flux values (value-predicting models). These can be validated by correlating predictions with observations in the test dataset. Another method of evaluation is to identify flux events (e.g., $\geq \%75th$ or 90th percentiles) and categorize output predictions into above or below these cut offs. The ability of the model to distinguish event from non-event can then be assessed with a Heidke skill score (see below for calculation details) which compares predictions to a null hypothesis of random assignment to classes.

4 Assessing the Value-Predicting Models

4.1 Assessing the 40 keV ARMAX models

We start our analysis with predictions of 40 keV electron fluxes. Figure 1 presents the predictions of the observed (shown in blue) 40 keV electron fluxes using the base AR-MAX model over the training set (shown in green) and the validation period (shown in orange). (To facilitate comparison of the influence of predictors with widely different units, we use Z-scores obtained by subtracting the mean of each series and dividing by its standard deviation.) The base ARMAX model validation r = 0.731 appears to give a reasonable fit to observations in the validation (test) set. The training set r = 0.819, when squared, gives an $R^2 = 0.670$, showing that a reasonable fraction (67.8%) of the variability is captured by the ARMAX model. (The R^2 is mathematically equivalent to the prediction efficiency, or PE, used in some other work.) However, a timeplot of observed and expected points reveals that the model does a poor job of predicting the high and low extremes in the validation set compared to the training set (Figure 1).

Figure 2 shows a more detailed view of just the validation period. Predicted values from the base ARMAX model do follow the general rise and fall of observed flux (Figure 2a; further metric scores are given in Figure 4 and Table 2. However, this expanded view shows more clearly that the base model has more trouble predicting high values than low values. Adding Lag 1 flux (40 keV flux from the previous hour) as a predictor provides some improvement (Figure 2b; validation r = 0.822), but we will discuss below why this is not an optimal approach.

The model is improved in both validation correlation (0.804) and apparent ability to predict highs and lows by adding MLT as a categorical variable to account both for the differing levels of flux and the differing response of flux to the other predictors throughout the diurnal period (Figure 2c; ARMAX-MLT model). An improvement in validation correlation (0.859) can be achieved by adding 40 keV flux from 1 h previous (Lag 1 flux) as a predictor to the ARMAX-MLT model (Figure 2d). Less improvement (validation r = 0.814) is seen if 40 keV flux 6 h previous (Lag 6 flux) is added instead (Figure 2e).

However, further assessment of these models at a finer scale reveals that adding previous flux from an hour before as an explanatory variable, while increasing the validation correlation, causes predictions to lag behind observations. Figure 3 shows the predictions over one week of the validation period (6-12 December 2016). The base ARMAX

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Figure 1. Predictions from the Base ARMAX model (40 keV) over the training set (predictions in green) and the validation period (predictions in orange). Flux is converted to unitless Z-scores.

Observed.

Predicted



Figure 2. Predictions over the validation period (40 keV) from a. Base ARMA model, b. ARMAX-MLT, c. ARMAX-MLT with flux at lag 6 added as a predictor, d. ARMAX-MLT with flux at lag 1 added as a predictor, e. ARMAX-MLT with flux at lag 6 added as a predictor. Flux is converted to unitless Z-scores. Further metrics are given in Figure 4 and Table 2.

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model prediction tracks the pattern of the observations, although always lower at the peaks (Figure 3a). Adding the Lag 1 flux to the base ARMAX model appears to track the height of the peaks better and to improve the validation correlation (0.822), but visually we can see that these predictions lag behind by 1 h (Figure 3b). This results in predictions that appear very good, but only an hour after we already know what the flux was. More quantitatively, we can assess models for this delay problem by comparing the same time vs. the Lag 1 validation correlation. In the model including Lag 1 flux, the correlation between observations and the prediction 1 h later (0.978) is much higher than between observation and prediction from the same time step (0.822). In contrast, the Lag 1 validation for the base ARMA model is lower than the same time validation. Note that this delay in prediction is only due to the introduction of Lag 1 flux, as all other parameters are the same between these two models.

Over this one week, the ARMAX-MLT model tracks the observed peaks somewhat better, without a delay (the overall Lag 1 validation is lower than the same time validation) (Figure 3c). Adding Lag 1 flux to the ARMAX-MLT model does not as obviously introduce a delay in this one week, but over the entire test period, the Lag 1 validation correlation is still slightly higher than the same time validation (Figure 3d). Although the ARMAX-MLT+Lag1Flux model does appear to somewhat improve the ability to reproduce the peaks, we cannot guarantee that flux from one hour previous would be available for real time forecasting. However, the more important shortcoming is that we are likely most interested in those occasions when flux rises sharply and unexpectedly. The very predictions we are most interested in are the ones that will fail to be predicted until an hour after the occurrence.

We consider a compromise model, the ARMAX-MLT+Lag6Flux model (Figure 3e), in hopes that this will predict peaks better but without the disadvantage of a delay. However, while this does not show a delay in predictions (same time validation r = 0.814vs Lag 1 validation r = 0.765), the overall validation correlation of 0.814 is not much above the ARMAX-MLT model alone (0.804), and peak prediction is not improved.

Thus, of the ARMAX models at 40 keV, the ARMAX-MLT is the best model in that it correlates reasonably well with observations and does not show a delay. However, we would hope for a model that is able to predict the peaks better.

4.2 Validation of 40-150 keV ARMAX Models

Scatterplots of observations vs. predictions from several ARMAX models give more information (Figure 4). We use scatterplots, rather than 2-D density plots, because the most important information (the over and under prediction of the low and high flux) is contained in the areas of lowest point density. Using 40 (column of three plots in Figure 4a), 75 (column of three plots in Figure 4b) and 150 keV (column of three plots in Figure 4c) electron fluxes, only over the validation period, we show a number of diagnostics. In each plot, the red line shows the ideal 1:1 relationship between prediction and observation. Many of the scatterplots not only show a great deal of scatter around this idealized 1:1 line, but also non-linearity between observed and predicted values. Points above the red line in the lower left or below the red line in the upper right represent predictions that failed to reach the lows and highs, respectively, in the observed data. The orange line is the cubic fit to these deviations and can be used to roughly assess how serious this problem is for each model. In the best case, the orange cubic line would lie on the 1:1 line, showing a model that reproduced the peaks and valleys well. The base AR-MAX model at 40 keV is a model that does particularly poorly at this task. The orange cubic fit in this case veers radically from the 1:1 red line. Both valley and peak magnitudes are severely under-predicted.

We report RMSE (root mean square error, or the standard deviation of the prediction vs observation residuals over the test set), and the MAE (mean absolute error,



Figure 3. Predictions over 1 week of the validation period (40 keV) showing how the models incorporating Lag 1 flux lag behind observations. a. Base ARMA model, b. Base ARMA with lag 1 flux, c. ARMAX-MLT, d. ARMAX-MLT with flux at lag 1, e. ARMAX-MLT with flux at lag 6. Flux is converted to unitless Z-scores. Lag 1 validation r correlates current observations with the prediction one hour previous. Models with Lag 1 flux as a predictor have higher Lag 1 validation correlation than same time validation correlation.





Figure 4. Scatterplots of predictions vs. observations over the full validation period and all three energies (a. 40 keV, b. 75 keV, c. 150 keV). Row 1: Base ARMA model, Row 2: ARMA model split by MLT (ARMAX-MLT), Row 3: ARMAX-MLT with lag 6 flux added as an additional predictor. Red line shows the ideal 1:1 correspondence between predictions and observations. Orange line gives the cubic fit to the actual prediction-observation relationship. Flux is

converted to unitless Z-scores. This article is protected by copyright. All rights reserved. **Table 2.** Median symmetric accuracy (MSA) and symmetric signed percentage bias (SSPB)

 metrics for the value-predicting models (built on Z-score transformed data).

| Base ARMAX ARMAX-MLT ARMAX-MLT+Lag6 | 40 keV MSA 5.70% 5.00% 5.00% | SSPB -0.20% -0.80% -0.80% | 75 keV MSA 4.10% 3.80% 3.80% | SSPB -0.70% -1.20% -1.20% | 150 keV MSA 4.00% 3.70% 3.70% | SSPB -1.50% -1.40% -1.90% |
|---|--|------------------------------------|--|------------------------------------|---|------------------------------------|
| REG-MLT | 5.10% | -0.40% | 3.90% | -0.80% | 4.00% | -1.10% |
| Base RNN RNN-MLT | $5.40\% \\ 4.90\%$ | -0.70% -0.10% | $3.70\%\ 3.70\%$ | -0.10% -0.004% | 3.30% 3.20% | -0.80% -0.10% |

or the average of the absolute differences between prediction and observation). The MAE is less sensitive to outliers, as the differences are not squared. (It is the same measure as the MAD, or mean absolute deviation.) Bias is the average of the differences of prediction and observation, without taking the absolute value. This measures whether predictions tend to lie above or below the observations. All these measures will indicate better fit when they are lower in magnitude (Hyndman & Athanasopoulos, 2018). Note that the standard deviation of the datasets is the same for all models as all use the same data (with standard deviation = 1 as these are Z-scores). Additionally, we calculate median symmetric accuracy (MSA) and symmetric signed percentage bias (SSPB) metrics (Table 2) (Morley et al., 2018). These two metrics appear to improve on the commonly used MAPE (mean absolute percentage error, which we do not use) by reducing the influence of outliers. However, this assumes that outliers do not carry relevant information, and in the case of our models, it is the points lying outside the main cloud that are of most interest to us, both because they lie in the regions of most interest (high or low flux) and because it is important to flag these areas where the predictions fail. Metrics based on the median of the error (MSA) reduce the influence of the error outliers, the rarer situations where the model performs the worst. RMSE, based on the mean of the errors, is more influenced by outliers and is therefore the more appropriate metric for assessing model failures. As MSA and SSPB use the ratio of prediction to observation rather than the difference, they may be better for data where the error variance increases or decreases with magnitude (heteroscedasicity) (Tofallis, 2015). However, as we have already dealt with the increasing error variance problem by taking the log and then the Z-score of the variables, the use of these metrics is redundant in that regard.

We should also point out a potential difficulty of MSA and SSPB with our particular data set. As these two metrics take the log of the ratio between observation and prediction, which can be negative if the data is transformed by log or Z-score, it was necessary to further transform the data by moving both observation and prediction above zero by adding the magnitude of the lowest observation. It is unclear to us if this transformation changed the behavior of this metric. However, the inability of the MSA and SSPB to distinguish between our value-predicting models (see Table 2) mean that these metrics are of limited use in this situation beyond demonstrating that the mid-range bulk of observation-prediction pairs are forecast well.

At all three flux energies, the ARMAX-MLT model, with higher validation correlation (0.769–0.804) and slightly lower RMSE, MAE, and MSA, improves on the base ARMAX models (r = 0.731 - 0.749). However, the ability to predict highs and lows correctly (comparing orange cubic line to red 1:1 line) is only slightly improved. The differences between ARMAX-MLT and ARMAX-MLT+Lag6 are not appreciable. The clear choice, for simplicity, would be the ARMAX-MLT model.

4.3 Validation of the Value-Predicting RNN Models

We would hope that a neural network model, by efficiently utilizing all available information in the data, would produce a prediction that both improved on the validation correlation and was more successful at predicting highs and lows. By building a time series dependent model using RNN (which we base on the previous 48 hours of predictor values), we also expected this would model the behavior of flux over time as well the ARMAX models. However, despite how the RNN model should include both this time dependent behavior and possible nonlinear information, we find no or, at best, only modest improvements in validation r (0.751–0.753), compared to the ARMAX models (Figure 5). Creating a separate model for each MLT does result in a small improvement over the base RNN model, but the metrics (validation r, RMSE, MAE, and MSA) are not much different from those of the ARMAX-MLT model.

4.4 Validation of the Reduced Polynomial/Interaction Regression Models

We are also interested in whether a parsimonious, more portable model, could be produced by ignoring the time series behavior of flux and focusing solely on the linear and nonlinear associations of flux with the predictors. This could work well if the time behavior of electron flux was highly dependent on the time behavior of the predictors. Nonlinear associations could take the form of multiplicative interactions (flux responding to each predictor differently depending on the levels of the other predictors), or some sort of polynomial response (quadratic, cubic, etc.). The possibility also exists that a long time stretch of predictors is not needed to produce a reasonable model. Predictors from a single or several hours before may be sufficient.

We created models containing all multiplicative interaction terms between predictors from one hour previous, as well as linear, quadratic, and cubic terms for each. We also included MLT as a categorical variable, including its interaction terms with the continuous variables. We label these as the REG-MLT models. However, adding all these terms resulted in unstable models that would be unsuitable for predictive purposes, so we further used stepwise regression (Neter et al., 1990) to trim the models down to the terms that best described flux. The stepwise process removed all cubic terms, leaving only linear, quadratic, and multiplicative interaction terms. These models, with validation correlation of r = 0.745 - 0.777, do only slightly worse at prediction, comparing the validation correlations, than the ARMAX-MLT models (Figure 6). As with the ARMAX-MLT models, there is also a tendency to underpredict the highs and over predict the lows, as evidenced by the cubic fit (orange line). RMSE, MAE, MSA, and bias measures are also similar to the ARMAX-MLT model. The advantage of this REG-MLT approach, however, is that these models would be more easily implemented by other users as all that is needed, after converting the data to standardized Z-scores, are the coefficient terms of the regression. While a neural network is also just a set of coefficients, the number of terms needed will be much lower for the stepwise-reduced REG-MLT model if statistically non-significant parameters are removed. This means that future prediction would be dependent on fewer inputs. Extraction of these coefficients is also easier as the output from a regression model in most statistical packages is simply the labelled coefficients. In the specific models we present here, there also appears to be little predictive advantage in including terms that describe time behavior, either the AR and MA terms of the ARMAX models or the 48 h measurements leading up to the flux prediction in the RNN models.

The validation correlation coefficients of the value-predicting models are all fairly close, but at 40 keV, the ARMAX-MLT model has the highest correlation with observations in the test set (Figure 7). At 150 keV, however, the 95% confidence intervals overlap so closely that there is no statistical difference between the models.



Figure 5. Scatterplots of predictions vs. observations for RNN models over the full validation period and all three energies (40 keV - 150 keV). First row: Base RNN model, second row: RNN-MLT. Red line shows the ideal 1:1 correspondence between predictions and observations. Orange line gives the cubic fit to the actual prediction-observation relationship. Flux is converted to unitless Z-scores.



Figure 6. Scatterplots of predictions vs. observations for the REG-MLT model over the full validation period and all three energies (a. 40 keV, b. 75 keV, c. 150 keV). Red line shows the ideal 1:1 correspondence between predictions and observations. Orange line gives the cubic fit to the actual prediction-observation relationship. Flux is converted to unitless Z-scores.



Figure 7. Validation correlation coefficients of the value-predicting models (base ARMAX, ARMAX-MLT, base RNN, RNN-MLT, and REG-MLT). Although 95% confidence intervals around each correlation are small, there is little practical difference between the models using this metric.

| | | a. Z-score of | | | b. Log10 Flux | | | c. Untransformed | |
|--------------|--------|---------------|---------|---------------------|---------------|---------|--------|------------------|---------|
| | | Log10 Flux | | | | | | Flux | |
| | 40 keV | 75 keV | 150 keV | $\mid 40~{\rm keV}$ | 75 keV | 150 keV | 40 keV | 75 keV | 150 keV |
| | | | | | | | | | |
| RMSE | 0.65 | 0.66 | 0.66 | 0.27 | 0.26 | 0.28 | 70944 | 33235 | 7118 |
| MAE | 0.49 | 0.47 | 0.47 | 0.19 | 0.19 | 0.2 | 30997 | 13314 | 3320 |
| Bias | 0.04 | 0.07 | 0.06 | 0.02 | 0.03 | 0.02 | 16719 | 7590 | 1640 |
| MSA | 5.10% | 3.90% | 4.00% | 3.20% | 3.30% | 4.00% | 39.00% | 37.90% | 40.70% |
| SSPB | -0.40% | -0.80% | -1.10% | -0.30% | -0.60% | -1.00% | -0.01% | -0.10% | 0.13% |
| | | | | | | | | | |
| validation r | 0.777 | 0.766 | 0.746 | 0.777 | 0.766 | 0.746 | 0.777 | 0.766 | 0.746 |
| | | | | | | | | | |
| Flux Std Dev | 1.026 | 1.023 | 0.983 | 0.426 | 0.405 | 0.417 | 95060 | 40636 | 9025 |
| RMSE/StdDev | 0.6335 | 0.6452 | 0.6714 | 0.6338 | 0.6421 | 0.6715 | 0.7463 | 0.8179 | 0.7887 |

Table 3. Metrics of the REG-MLT models calculated from a. Z-score standardized flux, b.log10 flux, and c. original flux units.

Using the REG-MLT models, we take the opportunity to compare metrics for standardized (Z-score of log10 flux) and backtransformed non-standardized (Log10 flux), and the completely backtransformed flux data (Table 3). First, the RMSE is strongly influenced by the standard deviation of the response variable. The standard deviation of the three $(\log 10)$ electron energies are all near 0.4 while that of the Z-score fluxes are roughly 1. (The standard deviation of the standardized test set is close to but not exactly 1 because the original standardization values were calculated from the training set.) Because the RMSE scales with the standard deviation, the unstandardized RMSE metrics are less than half the RMSE of the standardized output. This gives the erroneous impression that the unstandardized flux produces a better prediction. However, the untransformed flux data, with standard deviation in the 10^4 range, has a similarly large RMSE. This clearly demonstrates that we should not directly compare the RMSE metric between models using differently scaled data. We can standardize the RMSE by dividing by the standard deviation, as shown in the table (Liemohn et al., 2021). The other metrics are also affected by the scaling difference. The MSA, although it does not scale strictly linearly with the standard deviation, still shows a huge difference among the same predictions that merely differ in units, but the MSA is not as easily scaled to the standard deviation. Only the validation correlation is unaffected by changes in standard deviation or units. However, all these metrics are weighted heavily by the accurate prediction of mid-range values, missing the high and low values that are of most interest.

4.5 Prediction above a Threshold

Another method of comparing model accuracy is to determine how often models correctly predict a flux rise over a certain threshold, with correct predictions being true positives (TP) and true negatives (TN) and incorrect predictions being false positives (FP) and false negatives (FN). These four categories can be used to calculate an accuracy rate:

$$ACC = \frac{TP + TN}{TP + TN + FP + FN} \tag{1}$$

The true positive rate (TPR = TP/(TP+FN)) gives the rate at which surpassing the threshold is correctly predicted. The true negative rate (TNR = TN/(TN + FP)) is the proportion of the time the model correctly predicts that the flux will stay

below the threshold. The false positive rate (FPR = 1 - TNR) is the misses due to predicting over the threshold when the observation stays below, and the false negative rate (FNR = 1 - TPR) the rate at which it is predicted flux will stay below the threshold when, in fact, it goes above it (Yerushalmy, 1947).

The TP, TN, FP, FN, and ACC can be compared directly, or used to calculate the Heidke Skill Score (HSS) (Heidke, 1926). A score below zero will be obtained if the model predicts less well than chance alone. Scores closer to 1 show greater accuracy in prediction, with a score of 1 representing a perfect prediction:

$$HSS = \frac{2(TP \times TN - FP \times FN)}{[(TP + FN)(FN + TN) + (TP + FP)(FP + TN)]}$$
(2)

We calculate the HSS for several of the above models, predicting above either the 75th or 90th percentile (Table 4). Based on the HSS, the REG-MLT model appears to be more accurate than any of the ARMAX models, but less accurate than the RNN models This is a different ranking of models than that obtained from the validation correlations where the ARMAX models did better. However, these differences are small and are likely not of much consequence. In general, but not always, these models perform somewhat better in predicting flux above the 75th percentile than above the 90th percentile.

These skill scores are higher than those obtained by Ganushkina et al. (2019) for flux events predicted by the IMPTAM (Inner Magnetosphere Particle Transport and Acceleration Model), the highest skill score being 0.17 for the 40 keV electrons at roughly the 75th percentile. Although, this previous study was predicting events at 10 minutes, a more difficult task, much of this difference in skill scores may be due to our use of a strictly empirical model and the incorporation of MLT both as a predictor in its own right and as a modifier of the other variables which may behave differently at different times or locations. A NARMAX model predicting daily averages of higher energy electron flux (≥ 2 MeV) achieved a Heidke skill score of 0.738 (Balikhin et al., 2016). Our ARMAX, REG-MLT, and RNN results for hourly lower energy electrons are somewhat lower than this, reflecting the that the prediction of both hourly flux and lower energy flux are more more difficult task.

5 Building Probability Prediction Models: RNN and Logistic Regression

If we are interested in predicting above a threshold (e.g., a certain percentile) we may find that a probability model, rather than a value-predicting model, may give us more accuracy. Both regression and neural network models, such as RNN, can be made to output the probability of being above a threshold rather than a specific value. A regression of this sort is called logistic regression (Neter et al., 1990; Berkson, 1944). We classify flux observations and predictions $\geq 75th$ percentile as an event. Those less than this cut off are a non-event. (Note that this percentile is not the same as the probabilities discussed in the next paragraph.) Previously, this approach (used for daily predictions) was found to be more accurate at predicting events than value-predicting multiple regression or ARMAX models (Simms & Engebretson, 2020). We create several models using these algorithms: RNN-MLTclass (a series of RNN models, one for each MLT, classifying predictions into the event and non-event groups); LogisticLag1, LogisticLag3, and LogisticLag6 (all including MLT and each using predictors from 1, 3, or 6 hours before the flux measurement).

But at what probability do we forecast an event? A threshold of probability = 0.5 can be used as a default value (equal probability of either outcome), but there is generally a more optimal cut off point which can be determined from either a ROC (receiver

operating characteristic) curve (Fawcett, 2006; Liemohn et al., 2020, 2022), or from a precision-recall curve, which is thought to often provide better accuracy for rare events (Saito & Rehmsmeier, 2015). A ROC curve plots TPR vs FPR and highlights the ability of the model to distinguish between the two classes. Alternatively, precision (TP/(TP+FP)) vs. recall (TPR) plots better highlight the ability to accurately detect events, particularly if they are rare. The threshold point of either curve can be "tuned" to find the optimal cut off for distinguishing between classes by finding the maximum accurate separation between the classes.

RNN naturally incorporates past values of predictors if needed (we have chosen to use up to 48 hours from past predictor values). If these past values are important, we expect that a logistic regression based on only one previous time step would not do as well as an RNN model. Although we could enter many time steps into the logistic regression, we found that more than one either resulted in a model that could not converge, or provided very little further explanation of the variance. Using a stepwise procedure, as in the REG-MLT model above, cubic terms were not found to be useful. The variables in the logistic models, therefore, included only a single previous time step (Lag 1, 3, or 6), and whichever main effects, interactions, and quadratic terms were chosen as influential by the stepwise procedure.

We report the usual true and false positive rates (TPR or hit rate, and FPR or false alarm ratio), true and false negative rates (TNR and FNR), along with the AUC (area under the ROC curve), the Heidke skill score (HSS), Matthews correlation coefficient (MCC), and the critical success index (CSI) all at the optimal threshold determined from a precisionrecall curve (Table 5). (See Chakraborty and Morley (2020) for CSI and MCC calculations.) The AUC is often used to compare models. A larger area under the ROC curve corresponds to a model that better differentiates between classes, with a value of 1 being completely accurate discrimination. All the AUC values, for both logistic and RNN models, are similar (0.850 - 0.907). Based on the AUC values alone, we could conclude that all models are performing well and roughly equally, but other metrics may also be considered. The HSS, MCC, and CSI measure somewhat different attributes: the improvement over random forecasts (HSS: Heidke (1926)), a measure of correlation of classes unaffected by unbalanced data (MCC: Chicco and Jurman (2020)), or a measure weighted to give more value to warnings for rare events (CSI: Schaefer (1990)). The Heidke skill scores lie within a small range (0.557 - 0.667), so although the 95% confidence intervals from 10,000 bootstrap resamplings of the data (of size 7000 points) of the HSS for each of these models is small, there is still considerable overlap between models (Figure 8). (Overlap of the 95% confidence intervals is equivalent to finding no difference between means in a t-test.) The ranges of MCC (0.558 - 0.673) and CSI (0.537 - 0.684) are similarly narrow and therefore also do not provide much discrimination between models. We do not show the bootstrap assessments of the MCC and CSI variation as they were also very small. (Bootstrapping randomly resamples, with replacement, from the original sample to obtain a standard error needed to create confidence intervals or perform hypothesis tests for statistics for which the underlying distribution is not otherwise known (Efron & Tibshirani, 1986))

Although the LogisticLag6 model consistently performs worse in all these metrics, there is no particular advantage to the RNN-MLTclass models over the LogisticLag1 or LogisticLag3. Again, this suggests that the RNN algorithm is not adding anything more than what we have incorporated into the logistic models. We may as well use the more portable model (the logistic model). Given that the LogisticLag1 and LogisticLag3 perform much the same, we would choose the LogisticLag3 (referred to as LL3 from now on) as the more practical model. Predictions could be made up to 3 h ahead instead of the 1 h required by all the other models we present.

For this one model (LL3; 150 keV) we show the determination of the optimal probability threshold using both the ROC curve and the precision-recall curve (Figure 9). With

the ROC curve, the optimal point on the curve is closest to the upper left corner (9a). (We determined this using the perfcuve function in MATLAB.) This gives an optimal probability threshold of 0.480, close to the "default" of 0.5. For the precision-recall curve, the optimal threshold is chosen by maximizing (Saito & Rehmsmeier, 2015):

$$2 \times \frac{Precision \times Recall}{Precision + Recall} \tag{3}$$

This gives an optimal threshold of 0.313 (Figure 9b). Although the overall accuracy (ACC of Equation 1) is slightly higher with the ROC optimal threshold (0.832 (Figure 9c) vs. 0.821 (Figure 9d)), the ACC can be quite high only because it identifies true negatives correctly without any correct identification of true events. For this reason, the ACC is often not the best measure. The Heidke skill score shows no improvement using the optimal threshold. It is 0.639 at the optimal point chosen by the precision-recall curve, but 0.646 at the point chosen by the ROC curve. There is some advantage in using the precision-recall curve point as there is an improvement in both the correctly predicted events (TPR) and a reduction in the number of missed events (FNR). There may be some tolerance for the increased false positives if it improves the true positive rate.

5.1 Predicting High Flux after Periods of Low Flux

If we choose the LL3 model as the most practical, predicting when flux will be above the 75th percentile 3 h later, there is one further test of its abilities we should make. As all these models are based on a dataset dominated by one quiet hour leading into another quiet hour, it would not be surprising if the ability to predict sudden rises were limited by the overwhelming number of quiet data points. Furthermore, all our identified models predict whether high flux will occur in the future without regard to the current status (low vs. high flux). It is a different task to predict a sudden rise in flux from a low level versus a persistence of high flux. This model type should be assessed for its ability to do that. In fact, we may find that a model made specifically for this situation would do a better job.

We created one more model (LogisticLag3red) which uses as its training set only those hours preceded by low flux. This removes all times when a high flux hour is preceded by high flux and gives us a method of predicting the specific case where flux rises from a lower level. We also test the ability of the original LL3 model to perform this same task by validating it only on the hours of the test set data which are preceded by low flux. This is a more difficult task: less than 7% of this reduced test set are hours of high flux following low flux. However, we find that these two models behave similarly, with the original LL3 model performing better (at 40 and 150 keV) or not much worse (150 keV) as measured by the Heidke skill score if the optimal threshold is moved to account for the lower percentage of observations in the event class (Table 6). The coefficients of the original LL3 (or LogisticLag3) model (Tables 7- 9) can therefore be used to predict this particular situation, if the revised optimal threshold coefficients are used (Table 10b), without the need for a specialized model for this situation. As expected, the HSS for these predictions are lower than the overall HSS from the LL3 model.

5.2 Using the LL3 Model for Prediction

We report the coefficients of the LL3 models (Table 7, Table 8, Table 9) for use in future predictions. Inputs into these models must be Z-scores of the solar wind, IMF, and geomagnetic index predictors, with logs taken as described above. For future reference, we use the LL3 (LogisticLag3) acronym for this model.

The MLT variable set consists of 23 indicator variables, one less than the number of MLT values ($MLT_0 - MLT_22$). The variable is discretized such that, for exam-



Figure 8. Heidke skill scores of the classifier models (LogisticLag1, LogisticLag3, LogisticLag6, and RNNclass-MLT). There is little difference between the models using this metric. Bootstrap confidence intervals (95%) are small.



Figure 9. Determining the optimal probability threshold (red circle) for the logistic Lag 3 (150 keV) model. a. ROC curve, b. precision-recall curve, c. classification of test set using the optimal threshold from ROC curve, d. classification of test set using optimal threshold from the precision-recall curve. Model predicts whether observation will be above or below the 75th percentile. AUC = area under the ROC curve, TPR = true positive rate, FPR = false positive rate, TNR = true negative rate, FNR = false negative rate.

 Table 4.
 Heidke skill scores for the ARMAX, stepwise regression (including MLT), and RNN

 regression models evaluated for their ability to predict flux above the 75th and 90th percentiles.

| | | $40~{\rm keV}$ | $75 \ \mathrm{keV}$ | 150 keV |
|----------------|---------------|----------------|---------------------|----------|
| Base ARMAX | 75th %ile | 0.586 | 0.597 | 0.622 |
| | 90th % ile | 0.386 | 0.488 | 0.535 |
| ARMAX-MLT | 75th %ile | 0.615 | 0.626 | 0.635 |
| | 90th % ile | 0.521 | 0.541 | 0.562 |
| ARMAX-MLT+Lag6 | 75th %ile | 0.613 | 0.624 | 0.634 |
| | 90th %ile | 0.518 | 0.546 | 0.566 |
| REG-MLT | 75th %ile | 0.625 | 0.636 | 0.619 |
| | 90th % ile | 0.570 | 0.591 | 0.549 |
| Base RNN | 75th %ile | 0.527 | 0.613 | 0.654 |
| | 90th %ile | 0.276 | 0.499 | 0.546 |
| BNN-MLT | 75th %ile | 0.602 | 0.638 | 0.663 |
| 101111-101121 | 90th %ile | 0.589 | 0.569 | 0.609 |

ple, MLT = 0 includes all observations where MLT = 0-0.99. An indicator variable is given the value of 1 for the hour it represents and 0 for all other hours. In other words, an observation at MLT 0 will have $MLT_0 = 1$, with all other MLT_0 variables = 0. An observation at MLT_23 is 0 in all MLT_ indicator variables.

The multiplicative interaction terms are produced by multiplying the relevant variables. Any multiplication between a numeric variable and an MLT indicator variable will result in 0 for all cases except the hour of the MLT.

Predictions are made with the usual regression equation:

$$Y_{pred} = b_0 + b_1 X_1 + \dots + b_n X_n \tag{4}$$

where b_0 is the constant term and each variable is multiplied by its corresponding coefficient $(b_1, ..., b_n)$, but the output must be converted back to probabilities:

$$Prob = \frac{e^{(b_0 + b_1 X_1 + \dots + b_n X_n)}}{1 + e^{(b_0 + b_1 X_1 + \dots + b_n X_n)}}$$
(5)

Once these probabilities are calculated, assignment to classes (above or below the 75th percentile) is accomplished by comparing to the optimal thresholds of Table 10a (Neter et al., 1990).

6 Discussion

Our exploration of various algorithms for creating predictive models shows that value predicting models (multiple regression, ARMAX, and RNN) have difficulty predicting the more extreme high and low fluxes of keV electrons at geostationary orbit. These models can be improved by including MLT, both as a term that describes the differing levels of flux over the 24 h period as well as how the influence of other predictors varies at

| Table 5. | Accuracy | metrics | for the cl | lassification | models: | logistic a | and RNN | -MLT |
|--------------|----------|---------|------------|---------------------|---------|------------|---------|------|
| Model | TPR | FPR | TNR | FNR | AUC | HSS | MCC | CSI |
| | | | | $40 \ \mathrm{keV}$ | | | | |
| RNN-MLTclass | 0.777 | 0.173 | 0.827 | 0.223 | 0.904 | 0.580 | 0.583 | 0.56 |
| LogisticLag1 | 0.813 | 0.154 | 0.846 | 0.187 | 0.907 | 0.632 | 0.636 | 0.60 |
| LogisticLag3 | 0.822 | 0.167 | 0.833 | 0.178 | 0.900 | 0.623 | 0.628 | 0.60 |
| LogisticLag6 | 0.716 | 0.151 | 0.849 | 0.284 | 0.85 | 0.557 | 0.558 | 0.53 |
| | | | | $75 \ \mathrm{keV}$ | | | | |
| RNN-MLTclass | 0.846 | 0.193 | 0.807 | 0.154 | 0.877 | 0.627 | 0.633 | 0.62 |
| logisticLag1 | 0.847 | 0.184 | 0.816 | 0.153 | 0.891 | 0.638 | 0.644 | 0.63 |
| LogisticLag3 | 0.828 | 0.155 | 0.845 | 0.172 | 0.903 | 0.657 | 0.659 | 0.64 |
| LogisticLag6 | 0.817 | 0.195 | 0.805 | 0.183 | 0.875 | 0.600 | 0.605 | 0.60 |
| | | | | 150 keV | | | | |
| RNN-MLTclass | 0.875 | 0.192 | 0.808 | 0.125 | 0.773 | 0.667 | 0.673 | 0.68 |
| LogisticLag1 | 0.846 | 0.197 | 0.803 | 0.154 | 0.871 | 0.636 | 0.639 | 0.65 |
| LogisticLag3 | 0.873 | 0.215 | 0.785 | 0.127 | 0.882 | 0.639 | 0.646 | 0.66 |
| LogisticLag6 | 0.855 | 0.191 | 0.809 | 0.145 | 0.883 | 0.650 | 0.654 | 0.66 |

Tclass.

ate (false prediction of an event); TNR: True Negative Rate (accurate prediction of non-event); FNR: False Negative Rate (false prediction of non-event). AUC: Area under the ROC curve.

Table 6. Classification model accuracy metrics when limited to periods when flux could increase above the 75th percentile.

| Model LogisticLag3red | TPR | \mathbf{FPR} | TNR | FNR | AUC | HSS |
|---|-------|----------------|-------|-------|-------|-------|
| Training set limited to starting low flux hours | | | | | | |
| 40 keV | 0.728 | 0.190 | 0.810 | 0.272 | 0.854 | 0.357 |
| 75 keV | 0.791 | 0.190 | 0.810 | 0.209 | 0.866 | 0.372 |
| 150 keV | 0.611 | 0.075 | 0.925 | 0.389 | 0.886 | 0.412 |
| LogisticLag3 | | | | | | |
| Training set includes all hours | | | | | | |
| 40 keV | 0.653 | 0.139 | 0.861 | 0.347 | 0.900 | 0.395 |
| 75 keV | 0.716 | 0.141 | 0.859 | 0.284 | 0.903 | 0.410 |
| 150 keV | 0.743 | 0.163 | 0.837 | 0.257 | 0.882 | 0.361 |

each hour (by the use of multiplicative interaction terms with the MLT variables). The addition of multiplicative interactions between inputs and of quadratic terms is helpful in the regression model. (Presumably, these are also added by the RNN algorithm although it takes some effort to determine this.) However, even with these additional terms highs and lows are still under reported. Adding Lag 1 flux as a predictor may appear to rectify the issue, but this results in predictions that lag an hour behind. This problem has also been found in a Kp predictive model. While adding historical Kp as a predictor improved the model, it resulted in missing rapid changes (Chakraborty & Morley, 2020). The addition of Lag 6 flux to our model, while it does not cause predictions to lag, also does not solve the problem of under-predicted highs and lows.

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The prediction of high flux following low flux is the most challenging task, but also of the most practical importance. Models trained on these full datasets can give excellent prediction of the status quo (either the common mid-range values or persisting flux) because they tend to predict best what they are most heavily trained on. To better predict just the start of high flux events, models can be built just on those days or hours when low flux could potentially rise to high flux (Simms & Engebretson, 2020). However, an increase from low to high flux is still a somewhat rare event (much less than 50%: 3049 out of 28921 hours or 10.5% of this subset) and without larger training sets, these empirical models may still struggle with predicting high flux events unless the relationship between flux increase and predictors is very strong. In fact, the high variability in flux response to the variables most often used for prediction might suggest that we are missing important parameters or processes that drive high flux events. One obvious candidate in our particular models is substorm activity as we cannot include the AE index if we intend to use a model for real time prediction. However, studies that have included the AE (see below) do not achieve better prediction.

The regression models (both conventional and logistic) are able to include main effects, multiplicative interactions, and quadratic and higher polynomial terms as needed. Thus, they could potentially produce a model very similar to that chosen by the RNN algorithm, with the exception that only a limited number of previous lags can be included before the model becomes intractable and too burdened with overly correlated predictors. The RNN models we created could, potentially, use up to 48 h of previous information, but limiting the number of previous hours in the regression models did not lower their predictive ability below that of the RNN models. We therefore conclude that the relevant prediction information is contained in the variables measured just an hour or up to 3 h before.

While cycling behavior may obscure the physical relationships of various processes, this may not be an issue with prediction models. For example, the nuisance diurnality of flux measurements from geosynchronous satellites may create misleading correlations. Models seeking to understand the physical drivers should account for this behavior, by such methods as ARMAX (autoregressive moving average transfer function) modelling or, at least, differencing of data to remove cycles (Simms, Engebretson, & Reeves, 2022), but perfectly serviceable prediction models can be produced even if these spurious correlations are not removed. Consequently, if ARMAX models are not needed to remove the cycling behavior, predictive models can be built from neural networks or simply from regression models. However, we must not make the mistake of interpreting an influential parameter in these latter methods as evidence that it is a physical driver of flux. We must recognize that the high correlation seen between some variables and flux in models that do not correct for co-cycling behavior and trends can only be interpreted as that parameter being a good proxy for the physical environment, not that that particular variable is the physical influence that drives electron flux. Bearing this in mind, when creating prediction models, we can choose an algorithm for model construction based on such constraints as predictive ability, ease of determination, and portability to other users rather than considerations of which parameters are physically responsible for driving flux.

We do want to introduce as many variables as needed to describe the behavior of flux, not merely choose the few that are most important. It is true that we are not interested in a cluttered model where there are many essentially duplicate variables, but previous work on drivers suggests that most available variables have some statistically significant association with flux even when other parameters are accounted for. Even if this apparent influence is small, there is little reason to discard a statistically significant variable. (The same does not hold true for a model seeking to answer questions about which variables are most likely to be drivers. As competition between variables can have large effects on both coefficient estimation and statistical testing, there are some sets of variables that should not be considered together in the same model.)

Model diagnostics should be geared to investigating the most important model failures. For value-predicting models, single metrics may not be the best choice. RMSE, MAE, bias, MSA, and SSPB showed only small differences and therefore were not able to differentiate between models well. Heavy weighting on the most numerous prediction-observation pairs in the middle range leads these metrics to discount serious errors in the more important, but less abundant, low and high flux ranges. This is the reason why we do not present 2-D density plots as they overlook the rarer, but more important, deviations from the model. Single metrics that seek to discount values farther from the predictions of the model, particularly if they are rarer, are even more misleading. The very low MSA values that we obtain (compared to RMSE and MAE) show that this outlier-protected metric is missing much of the reduced prediction ability that we need to assess. We also show that both the mean-based RMSE and the median-based MSA are highly influenced by the standard deviation of the response variable. Comparing these metrics over variables of different standard deviations is therefore meaningless. Response variables should be normalized to the same standard deviation before metric comparisons are made.

In this study, we have developed several techniques for assessing poor fit of the valuepredicting models that focus on the areas of most interest: the high and low fluxes. The first, the cubic fit line to the prediction-observation relationship, is a visual technique. Inspection of this line immediately tells us that the fit to highs and lows is much worse, for example, in the base RNN model than in the RNN-MLT model. The validation correlation only tells us that the fit is slightly worse and gives no indication of where the problem lies or how serious it is for our particular needs. Our second diagnostic, the Lag1 validation correlation, assesses whether the predictions lag behind the observations. While lagging in the mid-range values is not as problematic, the missing of large changes in flux until the hour after they have happened is more troubling. If the predictions correlate better with observations from the hour before than with the hour being predicted, this tells us that the model will be missing the events that we are most interested in. While including persistence (Lag1 flux) as a predictor creates an extreme case, it is possible that other predictors could produce the same behavior so this should be checked in future models.

Validation correlations of the 3 value-predicting model types are reasonable and all of about the same magnitude (ARMAX-MLT: 0.731 - 0.814; RNN-MLT: 0.683 - 0.753; REG-MLT: 0.745 - 0.777). There is no apparent advantage to any of these model building algorithms over the others in predictive ability. This suggests that each of these algorithms is accessing similar information from the predictors and that the choice of algorithm to build a model could depend mainly on accessibility. For a value-predicting model, a regression equation (the REG-MLT model) would be the obvious choice as there would be no need to transport the more complicated coefficients of an ARMAX or RNN model if the model were to be placed on another system.

The validation correlations we obtain are higher than the 0.67 validation correlation found for a previous hourly 40 keV ARMAX model (averaged over the individual MLT models) (Boynton et al., 2019). Reasons for this improvement in our ARMAX model may be that we include a decay term and that we create one, more efficient, model with

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indicator variables to identify the individual MLTs instead of a series of models for each MLT.

However, validation correlations are not the only way to assess such models. We may be interested in a model's ability to predict when flux will go over a certain threshold, such as the 75th percentile. In this case, we could evaluate models with the Heidke skill score, comparing the classification success against that of random assignment to categories. Using this metric, all 3 of these value predicting models perform similarly (Heidke skill scores at the 75th percentile of 0.615 - 0.635 (ARMAX-MLT), 0.602 - 0.663 (RNN-MLT), and 0.619 - 0.636 (REG-MLT)). All do better than random assignment and all are better than the output of the IMPTAM model where the highest skill score was 0.17 for 40 keV electrons at roughly the 75th percentile ((Ganushkina et al., 2019)). Although, this previous study was predicting events at 10 minutes, a more difficult task, much of this difference in skill scores may be due to our use of a strictly empirical model and the incorporation of MLT.

An ARMAX model (SNB^3GEO) predicting daily averages of higher energy electron flux (≥ 2 MeV at L=6.6) achieved a Heidke skill score of 0.738 (Balikhin et al., 2016). Our hourly models achieved a lower HSS, in part because hourly prediction is a more difficult task (Simms, Engebretson, & Reeves, 2022), and in part because correlations between predictors and lower energy flux are weaker. In our results, the 150 keV flux was usually somewhat better predicted than the 40 keV flux, so it is not surprising that 2 MeV electrons would be more easily predicted than the lower energies.

Another daily regression model (at L=5.2) using several solar wind parameters gave a correlation between model prediction and observation of 0.854 at > 900keV, although it is not clear if this is a true validation correlation (on a reserved test set) or a correlation on the training data which would naturally be quite high (Katsavrias et al., 2022). In this same study, a daily prediction neural network model built on data over a wide range of energies and L shells (33 keV - 4.062 MeV; L 2.6-5.6) visually showed good correspondence with observations from a test set, while prediction at L=6.6, on an out of sample dataset, appeared considerably worse. The same problem we have experienced of under predicting the high values appears at low electron energies, along with over prediction of the low values at > 0.8MeV.

The MERLIN model, a neural network model predicting 120-600 keV electrons, shows a Spearman's rho validation correlation of 0.8 (at 120 keV), however this model incorporates AE as a parameter, making it less useful for real time prediction (Smirnov et al., 2020)). This model also shows some difficulties with under predicting the highs and over predicting the lows. Although the validation correlation is reasonably high, this mostly represents accurate predictions in the less critical middle range. The ORIENT-M model, a neural network model for 50 keV - 1 MeV electrons, uses AE as a predictor as well (Ma et al., 2022). The R^2 0.45 – 0.7 on the withheld test dataset (1 month of data near L 6 for the 54 keV electrons) is therefore also not a good comparison to our model which does not incorporate the real time unavailable AE.

Predictions above or below a threshold can also be obtained from a dedicated classifier model such as logistic regression or a classifier RNN model. Our classifier models provided little improvement to the Heidke skill score metric above that of the value-predicting models and were also not much different from each other (RNN-MLTclass: 0.580 - 0.667; LL3: 0.623 - 0.657).

While the RNN models were given 48 h of previous variables to work with, the logistic regression models were given only predictors from 1, 3, or 6 h before. (Various combinations of 1 with 2, 3, 6 did not provide any improvement.) While the RNN models could, in principle, have used any combination of polynomial and interaction terms from any of the 48 h, we found that the stepwise procedure on the logistic models did not choose

any polynomial terms above a quadratic. Thus, while we did not investigate the details of which terms the RNN models chose, we feel confident that a single predictor lag (Lag 1 and Lag 3 worked best) and no polynomials above a squared term are sufficient to describe this data.

Classifier models may be a better choice if the goal is to predict when an event (flux above a threshold) will occur. Classifier neural networks may predict as well as logistic regression models, but the latter provide the most portability. The LogisiticLag3 model is preferred only because it would allow a 3 h lead in prediction time while not sacrificing any predictive power (as would be the case for the Lag 6 model). We therefore present the coefficients for the LL3 models (40-150 keV) in Tables 4-6 for future predictions.

We provide probability thresholds for classification using the LL3 model (Table 7) determined from optimizing precision vs. recall for two possible prediction scenarios: 1) predicting a flux over the 75th percentile from any flux level (high or low), and 2) predicting a rise in flux over the 75th percentile from a lower flux level. We found that it was not necessary to produce another model for predictions in the second scenario, that the optimal prediction could be obtained simply by moving the probability threshold. We assumed equal costs of missing the prediction of an event (a false negative) vs. predicting an event that did not happen (a false positive).

Finally, we note that what we have produced here are prediction models, not models showing physical dependence. Although there is overlap between which variables (and in what form) best predict flux and which may be physical drivers of flux, the variables chosen by the optimal prediction models are not necessarily those that have a physical influence on flux. First, we have limited our variables to those that can be accessed in real time so as to obtain useful predictions. While substorms (represented by the AEindex) may correlate well with flux this is not a useful variable for a working prediction model as AE is not available in real time. Second, as much of the correlation between predictor variables and flux is the result of common cycles (e.g., the diurnal cycle due to satellite position and the 27 d solar cycle; Simms, Engebretson, and Reeves (2022)), a good predictor may not be a driver at all. (For an investigation into the driving role of various parameters see Simms, Ganushkina, et al.) That the ARMAX models produced no better predictions than models derived by other means (RNN and regression) suggests that the description of the time behavior of flux can be accomplished either with AR and MA parameters or simply by using the co-cycling predictor variables, just so long as we have no reason to separate out the time behavior independent of these other variables. ARMAX modelling, therefore, is best suited to exploring actual physical relationships between flux and possible drivers, but does not give this model type any advantage in producing a predictive model. By the same argument, the coefficients of the regression models presented here are not any more interpretable in a physical sense than the hidden coefficients of a neural network, as we have not accounted for inflated correlations due to common cycles.

However, there is a more fundamental problem in confusing prediction models with models used to test hypotheses about physical relationships. If the model selection method depends on sorting through many possible models to find the "best" (this includes techniques such as neural networks and stepwise regression), the probability of rejecting a true null hypothesis becomes almost 100% and any conclusions based on this will be meaningless (Mundry & Nunn, 2009; Hurvich & Tsai, 1990; Whittingham et al., 2006). The result of this "many-models-choose-best" approach is that we have no firm basis to say anything about the probability that a particular variable chosen by this type of model is actually influential. This means that any attempt to determine the drivers of electron flux from the terms chosen by a many-models-choose-best approach is misguided. Even if the model predicts well, there is no basis for inferring that the particular variables chosen in the model selection phase have an actual physical influence.

7 Conclusions

1. We screen several algorithms for producing value-predicting models of hourly 40 - 150 keV electron flux at geostationary orbit: ARMAX, RNN, and regression. These methods produce roughly similar models, as measured by validation correlations and the Heidke skill score.

2. Classifier models (RNN and logistic regression) are somewhat better at predicting a flux event (flux rising above the 75th percentile) than value-predicting models. A model built by logistic regression using only variables from one previous time step predicts as well as one built by a neural network using 48 h of previous data. We choose the LL3 model because it is more parsimonious and more portable than an RNN model.

3. Although the prediction of high flux following a low flux hour is both the most difficult task as well as the most important, we were able to produce a reasonable prediction model for this special case merely by changing the probability threshold of the LL3 model.

4. Two new diagnostic tests are introduced to assess value-predicting models: the cubic fit to the observation-prediction relationship, to visually assess the degree to which high and low flux is under or over predicted, and the Lag1 correlation which determines the degree to which predictions may lag behind and miss rapid changes in flux. Additionally, to focus attention on the model failures instead of successes, we plot observations vs. predictions as scatterplots instead of 2-D density plots, the latter of which tend to discount the rarer but more important deviations from the model.

5. A "good" metric is one which focuses attention on the ability of a model to predict the cases of most interest, not simply one which produces a low value. We find that single metrics such as RMSE, MAE, bias, MSA, and SSPB are all too influenced by the bulk of well-predicted, mid-range values to differentiate between models that do better at predicting extreme values of flux. However, median-based metrics, such as the MSA, may be even less useful as they weight large deviations less heavily, giving an unreasonably reassuring picture of model effectiveness at predicting the outliers we are most interested in. We note that RMSE uses the prediction error mean, while the MSA (and SSPB) use the prediction error median. Use of the median in the MSA reduces the influence of prediction error outliers in the metric, thus it is of less use in identifying model failures than the RMSE is.

6. Single-value metrics such as RMSE (or MSA) which use the difference (or ratio) between observation and prediction are highly influenced by the standard deviation of the response variable. It is therefore meaningless to compare the RMSE or MSA across variables with different standard deviations. The Z-score transformation (obtained by subtracting the mean and dividing by the standard deviation) normalizes variables to a standard deviation of 1, making a comparison across models or datasets more useful.

7. Parameters are chosen for their availability, not solely due to their high correlation with flux. This is because we are interested in a useful model, rather than a model with the highest validation correlation. Some highly correlated variables (such as the AEindex) are not used because they would not be available in real time when predictions are needed.

8. The addition of MLT to these models, describing both the changing level of flux over the 24 h period as well as the change in predictor influence at each hour, improves predictions.

9. Value-predicting models do a poor job at predicting the highs and lows although mid-range prediction is very good. The relative rarity of data points in the areas of most interest (very high flux) results in models that will miss these events much of the time.

The addition of flux from the previous hour as an input variable appears to fix this problem, but produces predictions that lag behind observations.

10. The addition of multiplicative interactions between the predictor variables, as well as quadratic terms, improves predictions. Cubic terms had no effect.

11. Predictors from a full 48 h before are not needed. Variables measured in a single hour (1-3 h before the flux observation) are sufficient for a reasonable prediction. The time behavior of flux does not need to be described (i.e., with an ARMAX model) to produce reasonable predictions.

12. We provide coefficients and optimal probability thresholds to predict a flux rise above the 75th percentile 3 h in advance using a logistic regression model. (LL3) The logistic regression model was chosen for its portability to other systems. The 3 h time frame was chosen to provide a good balance between early warning and best prediction.

13. The best predictive model does not necessarily tell us anything about the physical relationship of each solar wind, IMF, or geomagnetic parameter with flux. If hypotheses about these relationships are to be explored, the model approach should be targeted to that goal instead of merely improving prediction scores.

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 Table 7.
 Coefficients of the 40 keV LL3 (Logistic Lag at 3 h) prediction model.

Constant -1.482 MLT Associated Coefficients:

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| В | -0.104 | | | MLT | $Bz \times MLT$ | $V \times MLT$ | $Kp \times MLT$ |
|------------------------|--------|---|-------------|--------|-----------------|----------------|-----------------|
| Bz | -0.542 | | MLT_0 | 0.275 | -0.009 | 0.046 | 0.047 |
| V | 0.418 | | MLT_1 | 0.375 | 0.040 | 0.040 | -0.052 |
| Р | 0.036 | | MLT_2 | 0.963 | 0.158 | 0.142 | -0.088 |
| Кр | 1.297 | | MLT_3 | 1.081 | 0.022 | -0.014 | 0.121 |
| Dst | -0.359 | | MLT_4 | 1.316 | -0.185 | -0.037 | 0.137 |
| B^2 | -0.092 | | MLT_5 | 1.079 | -0.200 | -0.145 | 0.500 |
| V^2 | -0.117 | | MLT_6 | 1.254 | -0.586 | 0.098 | 0.932 |
| $\mathbf{B} \times Bz$ | 0.065 | | MLT_{-7} | 1.203 | -0.496 | 0.322 | 0.374 |
| $\mathbf{B} \times V$ | -0.096 | | MLT_8 | 1.029 | -0.591 | 0.112 | 1.035 |
| $\mathbf{B} \times P$ | -0.065 | | MLT_9 | 0.650 | -0.417 | 0.176 | 0.944 |
| Bz $\times V$ | -0.083 | | MLT_{-10} | 0.679 | -0.485 | 0.022 | 0.480 |
| $Bz \times Kp$ | 0.229 | | MLT_{-11} | 0.359 | -0.214 | -0.318 | 0.896 |
| $V \times Kp$ | 0.272 | | MLT_12 | -0.291 | -0.093 | -0.133 | 0.973 |
| $P \times Kp$ | -0.224 | | MLT_13 | -0.387 | -0.237 | -0.080 | 0.288 |
| $Kp \times Dst$ | 0.184 | | MLT_14 | -0.752 | -0.127 | -0.366 | 0.347 |
| | | | $MLT_{-}15$ | -1.182 | -0.113 | -0.335 | 0.571 |
| | | | MLT_{-16} | -1.319 | -0.050 | -0.304 | 0.282 |
| | | | $MLT_{-}17$ | -1.973 | -0.225 | -0.292 | 0.360 |
| | | | MLT_{-18} | -2.563 | -0.301 | -0.198 | 0.753 |
| | | | MLT_19 | -2.169 | -0.274 | -0.176 | 0.538 |
| | | | MLT_20 | -1.632 | -0.070 | -0.067 | 0.614 |
| | | | MLT_21 | -1.572 | 0.111 | 0.079 | 0.635 |
| | | | MLT_22 | -0.473 | -0.060 | 0.231 | 0.016 |
| | | 4 | | | | | |
| | | | | | | | |
| | | | | | | | |

Table 8. Coefficients of the 75 keV LL3 (Logistic Lag at 3 h) prediction model.

| Constant | -1.986 | MLT Associated Coefficients: | | | | | | |
|-------------------------|--------|------------------------------|-------------|--------|----------------|-----------------|----------------|-----------------|
| В | -0.438 | | | MLT | $B \times MLT$ | Bz $\times MLT$ | $V \times MLT$ | $Kp \times MLT$ |
| Bz | 1.961 | | MLT_0 | 0.061 | 0.141 | -0.34 | 0.33 | -0.397 |
| Ey | 2.104 | | MLT_{-1} | 0.21 | -0.07 | -0.053 | 0.036 | -0.149 |
| V | 0.787 | | MLT_2 | 0.488 | -0.153 | 0.048 | 0.093 | 0.127 |
| Р | -0.085 | | MLT_3 | 0.863 | -0.077 | -0.114 | -0.1 | 0.179 |
| Кр | 1.432 | | MLT_4 | 1.199 | 0.167 | -0.332 | 0.07 | -0.074 |
| Dst | -0.797 | | MLT_5 | 1.355 | 0.17 | -0.397 | -0.111 | 0.201 |
| SolarFlux | -0.081 | | MLT_6 | 1.545 | 0.045 | -0.485 | 0.037 | 0.689 |
| B^2 | -0.07 | | MLT_7 | 1.663 | 0.118 | -0.485 | 0.229 | 0.463 |
| V^2 | -0.236 | | MLT_8 | 1.526 | 0.134 | -0.579 | -0.057 | 1.32 |
| P^2 | -0.081 | | MLT_9 | 1.29 | 0.422 | -0.388 | 0.023 | 0.501 |
| Kp^2 | 0.499 | | MLT_{-10} | 1.131 | 0.495 | -0.494 | -0.103 | 0.32 |
| $\mathbf{B} \times Bz$ | 0.118 | | MLT_{-11} | 0.793 | 0.318 | -0.328 | -0.046 | 0.991 |
| $\mathbf{B} \times V$ | -0.18 | | MLT_{-12} | 0.727 | 0.253 | -0.103 | -0.032 | 0.551 |
| $\mathbf{B} \times Kp$ | -0.349 | | MLT_13 | 0.456 | 0.444 | -0.256 | -0.024 | 0.164 |
| $\mathbf{B} \times Dst$ | -0.156 | | MLT_14 | 0.269 | 0.323 | -0.028 | -0.253 | 0.325 |
| $B \times SolarFlux$ | 0.084 | | $MLT_{-}15$ | 0.086 | 0.348 | 0.042 | -0.266 | 0.16 |
| Bz $\times V$ | 0.399 | | MLT_{-16} | -0.011 | 0.482 | -0.056 | -0.262 | -0.168 |
| $Bz \times P$ | -0.325 | | MLT_17 | -0.342 | 0.483 | 0.032 | -0.476 | -0.043 |
| Bz $\times Dst$ | -0.17 | | MLT_{-18} | -0.611 | 0.451 | -0.147 | -0.211 | -0.298 |
| Ey $\times P$ | -0.263 | | MLT_19 | -0.484 | 0.215 | -0.02 | -0.234 | -0.161 |
| Ey $\times Dst$ | -0.124 | | MLT_20 | -0.621 | 0.446 | -0.072 | 0.113 | -0.193 |
| $\mathbf{V} \times P$ | 0.071 | | MLT_21 | -0.838 | 0.358 | 0.044 | 0.03 | 0.152 |
| $V \times Kp$ | 0.226 | | MLT_22 | -0.592 | 0.392 | 0.026 | -0.07 | -0.114 |
| $V \times SolarFlux$ | -0.12 | | | | | | | |
| $P \times Kp$ | -0.183 | <u></u> | | | | | | |
| $P \times Dst$ | 0.133 | | | | | | | |
| $P \times SolarFlux$ | -0.093 | | | | | | | |

 $\mathrm{Kp} \times Dst$

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| Table 9. | Coefficients of the | 150 keV LL3 | (Logistic Lag at 3 h |) prediction model. |
|----------|---------------------|--------------|----------------------|---------------------|
|----------|---------------------|--------------|----------------------|---------------------|

| | | | Table 9. | Coefficier | ts of the 15 | 0 keV LL | 3 (Logistic Lag | g at 3 h) predie |
|-----------------|--------|----------|------------|-------------|--------------|----------|-----------------|------------------|
| Constant | -1.865 | MLT Asso | ciated Coe | efficients: | | | | |
| В | -0.533 | | | | | MLT | Bz X MLT | Kp X MLT |
| Bz | 0.773 | | | | MLT_0 | -0.395 | -0.039 | -0.105 |
| Ey | 0.718 | | | | MLT_1 | -0.400 | 0.305 | 0.045 |
| N | -0.146 | | | | MLT_2 | -0.048 | 0.246 | 0.086 |
| V | 1.130 | | | | MLT_3 | 0.166 | 0.273 | 0.189 |
| Кр | 0.309 | | | | MLT_4 | 0.656 | 0.078 | 0.282 |
| Dst | -1.098 | | | | MLT_5 | 0.954 | -0.053 | 0.250 |
| SolarFlux | -0.260 | | | | MLT_6 | 1.400 | -0.242 | 0.556 |
| B^2 | -0.121 | | | | MLT_7 | 1.603 | -0.097 | 0.579 |
| Bz^2 | -0.186 | | | | MLT_8 | 1.674 | -0.095 | 0.676 |
| N^2 | -0.094 | | | | MLT_9 | 1.619 | -0.066 | 0.699 |
| V^2 | -0.164 | | | | MLT_{10} | 1.562 | 0.073 | 0.778 |
| Kp^2 | 0.522 | | | | MLT_{-11} | 1.474 | -0.010 | 0.786 |
| Dst^2 | -0.057 | | | | MLT_12 | 1.260 | 0.072 | 0.574 |
| $SolarFlux^2$ | 0.009 | | | | MLT_13 | 1.086 | 0.106 | 0.445 |
| B:Ey | -0.111 | | | | MLT_14 | 0.819 | 0.223 | 0.461 |
| B:N | 0.093 | | | | $MLT_{-}15$ | 0.552 | 0.230 | 0.398 |
| B:V | -0.098 | | | | MLT_{-16} | 0.287 | 0.281 | 0.366 |
| B:Kp | -0.102 | | | | MLT_{-17} | 0.219 | 0.426 | 0.342 |
| B:Dst | -0.155 | | | | MLT_{-18} | -0.174 | 0.276 | 0.091 |
| B:SolarFlux | 0.185 | | | | $MLT_{-}19$ | -0.363 | 0.240 | 0.258 |
| Bz:Ey | -0.121 | | | | MLT_20 | -0.380 | 0.152 | 0.146 |
| Bz:Kp | -0.652 | | | | MLT_21 | -0.598 | 0.200 | 0.207 |
| Bz:Dst | -0.325 | | | | MLT_22 | -0.705 | 0.225 | 0.194 |
| Ey:Kp | -0.325 | | | | | | | |
| Ey:Dst | -0.228 | | | | | | | |
| N.Kp | -0.225 | | | | | | | |
| N:Dst | 0.303 | | | | | | | |
| N:SolarFlux | -0.073 | | | | | | | |
| V:Kp | -0.182 | | | | | | | |
| V:Dst | 0.182 | | | | | | | |
| V:SolarFlux | -0.183 | | | | | | | |
| Kp:Dst | 0.403 | | | | | | | |
| Dst:SolarFlux | 0.147 | Y | | | | | | |

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Table 10. Optimal thresholds for the LL3 prediction models, a. Using entire test set, b. Usingonly low flux hours that could rise above 75th percentile.

| Test set: | a. All hours | b. Starting low flux hours |
|---------------------|--------------|----------------------------|
| 40 keV | 0.34 | 0.17 |
| $75 \ \mathrm{keV}$ | 0.308 | 0.235 |
| 150 keV | 0.326 | 0.351 |

Acknowledgments

The work at the University of Michigan was partly funded by National Aeronautics and Space Administration grants NNX17AI48G, 80NSSC20K0353, and National Science Foundation grant 1663770. The contributions by M. van de Kamp and N. Ganushkina were also partly supported by the Academy of Finland (grant 339329). We thank the reviewers and editor (Dr. S. Morley) for their helpful suggestions.

Data Availability

The GOES-13 MAGED data and GOES Magnetometer 1 data used in the present study are available at https://www.ngdc.noaa.gov/stp/satellite/goes/dataaccess.html. Solar wind parameters and magnetic indices were obtained from OMNIWeb:

https://omniweb.gsfc.nasa.gov/form/dx1.html.

All models developed for this paper are available at doi:10.5281/zenodo.7520424.

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Figure Captions

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Figure 1. Predictions from the Base ARMA model (40 keV) over the training set (predictions in green) and the validation period (predictions in orange). Flux is converted to unitless Z-scores.

Figure 2. Predictions over the validation period (40 keV) from a. Base ARMA model, b. ARMAX-MLT, c. ARMAX-MLT with flux at lag 6 added as a predictor, d. ARMAX-MLT with flux at lag 1 added as a predictor, e. ARMAX-MLT with flux at lag 6 added as a predictor. Flux is converted to unitless Z-scores. Further metrics are given in Figure 4 and Table 2.

Figure 3. Predictions over 1 week of the validation period (40 keV) showing how the models incorporating Lag 1 flux lag behind observations. a. Base ARMA model, b. Base ARMA with lag 1 flux, c. ARMAX-MLT, d. ARMAX-MLT with flux at lag 1, e. ARMAX-MLT with flux at lag 6. Flux is converted to unitless Z-scores. Lag 1 validation r correlates current observations with the prediction one hour previous. Models with Lag 1 flux as a predictor have higher Lag 1 validation correlation than same time validation correlation.

Figure 4. Scatterplots of predictions vs. observations over the full validation period and all three energies (a. 40 keV, b. 75 keV, c. 150 keV). Row 1: Base ARMA model, Row 2: ARMA model split by MLT (ARMAX-MLT), Row 3: ARMAX-MLT with lag 6 flux added as an additional predictor. Red line shows the ideal 1:1 correspondence between predictions and observations. Orange line gives the cubic fit to the actual prediction-observation relationship. Flux is converted to unitless Z-scores.

Figure 5. Scatterplots of predictions vs. observations for RNN models over the full validation period and all three energies (40 keV - 150 keV). First row: Base RNN model, second row: RNN-MLT. Red line shows the ideal 1:1 correspondence between predictions and observations. Orange line gives the cubic fit to the actual prediction-observation relationship. Flux is converted to unitless Z-scores.

Figure 6. Scatterplots of predictions vs. observations for the REG-MLT model over the full validation period and all three energies (a. 40 keV, b. 75 keV, c. 150 keV). Red line shows the ideal 1:1 correspondence between predictions and observations. Orange line gives the cubic fit to the actual prediction-observation relationship. Flux is converted to unitless Z-scores.

Figure 7. Validation correlation coefficients of the value-predicting models (base ARMAX, ARMAX-MLT, base RNN, RNN-MLT, and REG-MLT). Although 95% confidence intervals around each correlation are small, there is little practical difference between the models using this metric.

Figure 8. Heidke skill scores of the classifier models (LogisticLag1, LogisticLag3, LogisticLag6, and RNNclass-MLT). There is little difference between the models using this metric. Bootstrap confidence intervals (95%) are small.

Figure 9. Determining the optimal probability threshold (red circle) for the logistic Lag 3 (150 keV) model. a. ROC curve, b. precision-recall curve, c. classification of test set using the optimal threshold from ROC curve, d. classification of test set using optimal threshold from the precision-recall curve. Model predicts whether observation will be above or below the 75th percentile. AUC = area under the ROC curve, TPR = true positive rate, FPR = false positive rate, TNR = true negative rate, FNR = false negative rate.

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Predicted Z Score







