



1 Analyses of different propagation models for the estimation of 2 the topside ionosphere and plasmasphere with an Ensemble 3 Kalman Filter

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9 Abstract.

10 The accuracy and availability of satellite-based applications like GNSS positioning and remote sensing crucially
11 depends on the knowledge of the ionospheric electron density distribution. The tomography of the ionosphere is
12 one of the major tools to provide link specific ionospheric corrections as well as to study and monitor physical
13 processes in the ionosphere and plasmasphere. In this work, we apply an Ensemble Kalman Filter (EnKF) approach
14 for the 4D electron density reconstruction of the topside ionosphere and plasmasphere with the focus on the
15 investigation of different propagation models and compare them with the iterative reconstruction technique
16 SMART+. The STEC measurements of ~~eleven~~ LEO satellites are assimilated into the reconstructions. We conduct
17 a case study on a global grid with altitudes between 430 and 20200 km, for two periods of the year 2015 covering
18 quiet to perturbed ionospheric conditions. ~~Particularly,~~ The performance of the methods to estimate independent
19 STEC and electron density measurements from the three Swarm satellites ~~is~~ ^{are} analysed. The results indicate that the
20 ~~methods~~ EnKF with ~~f~~ exponential decay as the propagation model and SMART+ perform best, providing ~~in~~
21 ~~summary~~ the lowest residuals.

22 1 Introduction

23 The ionosphere is the ~~upper~~ ^{charged} part of the atmosphere extending from about 50 - 1000 km and going over in the
24 plasmasphere. The characteristic property of the ionosphere is that it contains sufficient free electrons to affect the
25 ~~radio waves~~ propagation of trans-ionospheric radio signals, ~~as~~ from telecommunication, navigation or remote
26 sensing satellites, by refraction, diffraction and scattering.

27 Therefore, the knowledge of the three-dimensional electron density distribution and ~~their~~ ^{its} dynamics are of practical
28 importance. Around 50% of the signal delays or range errors of L-band signals used in GNSS originate from
29 altitudes above the ionospheric F2 layer, which consist of topside ionosphere going over into the plasmasphere.

30 So far, especially the topside ionosphere and plasmasphere is not well described. ^{reference for this} ~~bit 'clonky' should be reworded~~

31 The choice of the ionospheric correction model has an ~~essential~~ ^{major} impact on the accuracy of the estimated
32 ionospheric delay and its uncertainties. A widely used approach for ionospheric modelling is the single-layer
33 model, whereby the ionosphere is projected onto a two-dimensional ^(reference) spherical layer, typically located between
34 350 and 450 km. However, usually 2D models are not accurate enough to support high accuracy navigation and
35 positioning techniques in real time (e.g. Odijk 2002; Banville 2014). Additionally, they do not provide the
36 possibility to look insight the complex coupling processes between magnetosphere, plasmasphere and ionosphere.

37 More accurate and precise positioning is achievable by considering the ionosphere as 3D medium. There are
38 several activities in the ionosphere community aiming to describe the median ionospheric behavior by the

^{spell out first time}
^{Surely a 2D/3D model doesn't enable investigation of magnetospheric coupling. You need a full physics model for that. 2/D instead impacts bottomsides ionospheric uses such as HF propagation.}



39 development of 3D electron density models based on long-term historical data. Two widely used models are the
40 International Reference Ionosphere model (IRI, cf. Bilitza et al., 2011) and the NeQuick model (cf. Nava et al.,
41 2008).

42 Since those models represent a median behavior, it is essential to update them by the assimilation of actual
43 ionospheric measurements. There is a variety of approaches developed and validated for the ionospheric
44 reconstruction by combination of actual observations with an empirical or a physical background model.
45 Hernandez-Pajares et al. (1999) present one of the first GNSS-based data-driven tomographic models which
46 considers the ionosphere as a grid of three-dimensional voxels and the electron density within each voxel is
47 computed as a random walk time series. The voxel-based discretisation of the ionosphere is used for instance in
48 Heise et al., 2002; Wen et al., 2007; Gerzen and Minkwitz, 2016, Gerzen et al., 2017, Wen et al., 2020. These
49 authors reconstruct the 3D ionosphere by algebraic iterative methods. An alternative is to estimate the electron
50 density as a linear combination of smooth and continuous basis functions, like e.g. spherical harmonics (SPH)
51 (Schaer 1999), B-splines (Schmidt et al., 2008; Zeilhofer, 2008; Zeilhofer et al., 2010; Olivares-Pulido et al., 2019),
52 B-splines and trigonometric B-splines (Schmidt et al. 2015), B-splines and Chapman functions (Liang et al., 2015
53 and 2016), and empirical orthogonal functions and spherical harmonics (Howe et al., 1998).

54 Besides the algebraic methods, also techniques taking benefit of information on spatial and temporal covariance
55 information, such as Optimal Interpolation, Kalman Filter, three- and four-dimensional variational techniques and
56 Kriging, are applied to update the modelled electron density distributions, cf. Howe et al., 1998; Angling et al.,
57 2008; Minkwitz et al., 2015 and 2016; Nikoukar et al., 2015; Olivares-Pulido et al., 2019.

58 Moreover, there are approaches based on physical models, which combine the estimation of the electron density
59 with physical related variables such as neutral winds or the oxygen/nitrogen ratio (cf. Wang, et al. 2004; Scherliess
60 et al., 2009; Lee et al., 2012; Lomidze et al., 2015; Schunk, et al., 2004 and 2016; Elvidge and Angling, 2019).

61 In general, the majority of data, available for the reconstruction of the ionosphere and plasmasphere, are Slant
62 Total Electron Content (STEC) measurements, i.e. the integral of the electron density along the line of sight
63 between the GNSS satellite and receiver. Often, STEC measurements provide limited vertical information and
64 hence the modelling of the vertical the electron density distribution is hampered (Dettmering, 2003).

65 The estimation of the topside ionosphere and plasmasphere poses a particular difficulty since direct electron
66 density measurements are rare and since low plasma densities at these high altitudes contribute only marginally to
67 the STEC measurements. ~~E~~Especially, ~~G~~Ground-based STEC measurements are dominated by electron densities
68 within and below the characteristic F2 layer peak. Consequently, information about the plasmasphere ~~can be hardly~~ *is difficult to*
69 ~~extracted~~ *extracted* from ground-based STEC measurements, cf. e.g. Spencer and Mitchell, 2011. Thus, in ~~the presented~~ *this*
70 work, we concentrate on the modeling of the topside ~~part~~ *part* of the ionosphere and plasmasphere and utilize only ~~the~~
71 space-based STEC measurements.

72 In this paper, we introduce an Ensemble Kalman Filter to estimate the topside ionosphere and plasmasphere based
73 on space-based STEC measurements. The propagation of the analyzed state vector to the next time step within a
74 Kalman Filter is a ~~key point~~ *key challenge*. The majority of the approaches, working with EnKF variants, use ~~physic-based~~
75 models for the propagation step (cf. e.g. Elvidge and Angling 2019; Codrescu et al., 2018; Lee et al., 2012). In
76 our work, we investigate the question how the propagation step can be realized, if a physical model is not available
77 or if the usage of a physical model is rejected as computational ~~time consuming~~ *time consuming*. We discretize the ionosphere and
78 the plasmasphere below the GNSS orbit height by 3D voxels, initialize them with electron densities calculated by
79 the NeQuick model and update them with respect to the data. We present different methods how to perform the



80 propagation step and assess their suitability for the estimation of electron density. For this purpose, a case study
81 over quiet and perturbed ionospheric conditions in 2015 is conducted, investigating the capability of the
82 estimations to reproduce assimilated STEC as well as to reconstruct independent STEC and electron density
83 measurements.

84 We organize the paper as follows: Section 2 describes the EnKF with the different propagation methods and the
85 generation of the initial ensembles by the NeQuick model. Section 3 outlines the validation scenario with the
86 applied data sets and Section 4 presents the obtained results. Finally, we conclude our work in Section 5 and provide
87 an outlook on the next steps.

88 2 Estimation of the topside ionosphere and plasmasphere by EnKF

89 2.1 Formulation of the underlying inverse problem

90 The information about the slant total electron content (STEC), along the satellite-to-receiver ray path s can be
91 obtained from multi-frequency GNSS measurements. ~~In detail,~~ ^{The} STEC is a function of the electron density Ne
92 along the ray path s , given by

$$93 \quad STEC_s = \int Ne(h, \lambda, \varphi) ds, \quad (1)$$

94 where $Ne(h, \lambda, \varphi)$ is the unknown function describing the electron density values depending on altitude h ,
95 geographic longitude λ and latitude φ .

96 The discretization of the ionosphere by a 3D grid and the assumption of a constant electron density function within
97 a fixed voxel allows ~~us~~ the transformation of Eq. (1) into a linear system of equations

$$98 \quad STEC_s \approx \sum_{i=1}^K Ne_i \cdot h_{si} \Rightarrow y = Hx + r, \quad (2)$$

(1 would split these over
2 lines to make it easier to read)

99 where y is ^{an} ~~the~~ $(m \times 1)$ vector of the STEC measurements, x is the vector of unknown electron densities with $x_i =$
100 Ne_i equals the electron density in the voxel i , h_{si} is the length of the ray path s in the voxel i and r is the vector of
101 measurement errors assumed to be Gaussian distributed with $r \sim N(0, R)$ with expectation 0 and covariance
102 matrix R .

101 2.2 Background model

102 As regularisation of the inverse problem in Eq. (2), a background model often provides the initial guess of the
103 state vector x . In this study, we apply the NeQuick model version 2.0.2. The NeQuick model was developed at the
104 International Centre for Theoretical Physics (ICTP) in Trieste/Italy and at the University of Graz/Austria (cf.
105 Hochegger et al. (2000); Radicella and Leitinger (2001); Nava et al. (2008)). ~~We use~~ ^T the daily solar flux index
106 F10.7, ~~it~~ ^{it} drives the NeQuick model.

107 2.3 Analysis step

108 We apply an EnKF to solve the inverse problem defined in Section 2.1. Evensen (1994) introduces the EnKF as
109 an alternative to the standard Kalman Filter (KF) in order to cope with the non-linear propagation dynamics and
110 the large dimension of the state vector and its covariance matrix. In an EnKF, a collection of realisations, called
111 ensembles, represent the state vector x and its distribution.



112 Let $X^f = [x_1^f, \dots, x_k^f]$ be a $(K \times N)$ matrix whose columns are the ensemble members, ideally following the a priori
 113 distribution of the state vector x . Further, the observations collected in y are treated as random variables. Therefore,
 114 we define $\overset{an}{N}(m \times N)$ ensemble of observations $Y = [y_1, y_2, \dots, y_N]$ \in with $y_i = y + \epsilon_i$ and a random vector ϵ_i
 115 from the normal distribution $N(0, R)$.

116 We define the ensemble covariance matrix around the ensemble mean $E(X^f) = \frac{1}{N} \sum_{j=1}^N x_j^f$ as follows:

$$P^f = \frac{1}{N-1} \sum_{j=1}^N \left\{ (x_j^f - E(X^f)) \cdot (x_j^f - E(X^f))^T \right\}. \quad (3)$$

117 In the analysis step of the EnKF, the a priori knowledge on the state vector x and its covariance matrix is updated
 118 by

$$X^a = X^f + P^f H^T (R + H P^f H^T)^{-1} \cdot (Y - H X^f), \quad (4)$$

119 where the matrix X^a represents the a posteriori ensembles and hence the a posteriori state vector.

120 For the propagation of the analysed solution to the next time step, we test different propagation models described
 121 in Section 2.4. In order to generate the initial ensembles $X^f(t_0)$ we use the NeQuick model and describe the
 122 procedure in Section 2.5. Keeping in mind that we have to deal with ~~an huge~~ ^{extremely large} state vector (details are presented in
 123 Section 3.1), the big advantage of the EnKF, for the present study, is that there is no need for explicitly calculation
 124 of the ensemble covariance matrix (cf. Eq. (3)). Instead, to perform the analysis step in Eq. (4) we follow the
 125 implementation suggested by Evensen (2003).

126 2.4 Considered models for the propagation step

127 In this section, we introduce the different models investigated to propagate the analysed solution to the next time
 128 step. With all of them, we propagate the ensembles 20 minutes in time. These propagation models can be generally
 129 described as $X^f(t_{n+1}) = F(X^a(t_n)) + W_F(t_{n+1}) + \Omega_F(t_{n+1})$.

130 We applied different approaches to model F , the systematic error W_F and the process noise Ω_F and present in this
 131 paper a selection of the most promising variants of them.

132 2.4.1 Method 1: Rotation

133 The method Rotation assumes that in magnetic coordinates, the ionosphere remains invariant in space while Earth
 134 rotates below it (cf. Angling and Cannon, 2004). Thus, we propagate the analysed ensemble $X^a(t_n)$ from time t_n
 135 to the next time step t_{n+1} by:

$$X^f(t_{n+1}) = Rot(X^a(t_n)) + W_{rot}(t_{n+1}). \quad (5)$$

136 ~~In detail,~~ To calculate $Rot(X^a(t_n))$ the magnetic longitude is changed corresponding to the evolution time $\Delta t =$
 137 $t_{n+1} - t_n$, i.e. 5 degree of longitude per 20 minutes. W_{rot} denotes the systematic error introduced by approximation
 138 of the true propagation of X^f by a simple rotation. We tested here the following estimation of W_{rot} :

$$W_{rot}(t_{n+1}) = \overset{split\ over\ 2\ lines}{ratio_{rot}(t_{n+1})} \cdot E(Rot(X^a(t_n))) \cdot \epsilon_{1 \times N} \text{ and } ratio_{rot}(t_{n+1}) = \frac{(x^b(t_{n+1}) - Rot(x^b(t_n)))}{3 \cdot Rot(x^b(t_n))}, \quad (6)$$

139 where x^b is the electron density vector calculated by the NeQuick model and $\epsilon_{1 \times N}$ is an 1-by- N matrix of ones.

140 The division in the second equation is ~~an~~ element-wise ~~one~~.



141 **2.4.2 Method 2: Exponential decay**

142 Here we assume the electron density differences between the voxels of the analysis and the background model to
 143 be a first order Gauss-Markov sequence. These differences are propagated in time by an exponential decay function
 144 (cf. Nikoukar et al. 2015, Bust and Mitchell, 2008; Gerzen et al., 2015)

$$X^f(t_{n+1}) = X^b(t_{n+1}) \cdot \epsilon_{1 \times N} + f(t_{n+1}) \cdot [X^a(t_n) - X^b(t_n)], \quad (7)$$

145 where $X^b(t)$ is the ensemble of electron density vectors calculated by the NeQuick model for the time t as
 146 described in Section 2.5; $f(t_{n+1}) = \exp\left(-\frac{\Delta t}{\tau}\right)$; $\Delta t = t_{n+1} - t_n$; τ denotes the temporal correlation parameter
 147 chosen here as 3 hours.

148 Note: Similar to the method described here, we tested also the application of $Rot([X^a(t_n) - X^b(t_n)])$ instead of
 149 $[X^a(t_n) - X^b(t_n)]$ in Eq. (7). The results were similar and are therefore not presented here.

150 **2.4.3 Method 3: Rotation with exponential decay**

151 *For the* As third method, we define the propagation model as a combination of the propagation models described in the
 152 previous subsections, in particular

$$X^f(t_{n+1}) = x^b(t_{n+1}) \cdot \epsilon_{1 \times N} + f(t_{n+1}) \cdot Rot([X^a(t_n) - x^b(t_n) \cdot \epsilon_{1 \times N}]) + W(t_{n+1}) + \sqrt{\frac{\Delta t}{20}} \cdot \Omega_{exp}(t_{n+1}). \quad (8)$$

153 The systematic error W is estimated as *why 3/10?*

$$W(t_{n+1}) = f(t_{n+1}) \cdot \frac{3}{10} \cdot W_{rot}(t_{n+1}). \quad (9)$$

154 Thereby f and W_{rot} are defined as in the two *previous* sections ~~below~~. The process noise Ω_{exp} is assumed to be white with
 155 $\Omega_{exp}(t_{n+1}) = f(t_{n+1}) \cdot \Omega_{rot}(t_{n+1}) + (1 - f(t_{n+1})) \cdot Q_{exp}(t_{n+1})$. Here the matrix Ω_{rot} consists of random
 156 realizations of the distribution $N(0, \Sigma^{rot})$ with

$$\Sigma_{ii}^{rot}(t_{n+1}) = \left(ratio_i \cdot \left\{ E \left(Rot(X^a(t_n)) \right) \right\}_i \right)^2, \quad (10)$$

157 where $ratio_i$ increases continuously depending on the altitude of the voxel i from $\frac{0.5}{100}$ for lower altitudes to $\frac{1}{100}$ for
 158 the higher altitudes; $E \left(Rot(X^a(t_n)) \right)$ denotes the ensemble mean vector. The equations (8) and (10) can be
 159 interpreted as follows: for the chosen time step of 20 minutes, the standard deviation of the time model error

160 regarding the voxel i is equal to $\sqrt{\Sigma_{ii}^{rot}(t_{n+1})} = ratio_i \cdot \left\{ E \left(Rot(X^a(t_n)) \right) \right\}_i$, varying between 0.5% and 1% of
 161 the corresponding analyzed electron density in the voxel i . *In details, We* generate at each time step a new
 162 vector $\rho_i \sim N(0,1)$ with $\dim(\rho_i) = 100 \times 1$ and calculate *to calculate* the i -th row ω_i^{rot} of Ω_{rot} by

$$\omega_i^{rot}(t_{n+1}) = \sqrt{\Sigma_{ii}(\Omega_{rot}(t_{n+1}))} \cdot \rho_i(t_{n+1})^T. \quad (11)$$

163 The matrix $Q_{exp}(t_{n+1})$ consists of random realizations (different for each time step) consistent with the a priori
 164 covariance matrix L of the errors of the background $x^b(t_{n+1})$ (cf. Howe and Runciman, 1998). *In details, We* The a
 165 priori covariance is assumed to be diagonal and L_{ii} equals the square of 1% of the corresponding background
 166 model value. Then the i -th row of Q_{exp} is calculated by Eq. (12):

$$q_i(t_{n+1}) = \sqrt{L_{ii}(t_{n+1})} \cdot \rho_i(t_{n+1})^T. \quad (12)$$

I'm not sure where the matrix L has come from? Is the variable important or are you just giving the covar. matrix a name?



167 2.5 Generation of the ensembles

168 In order to generate the ensembles we vary the F10.7 input parameter of the NeQuick model (cf. Section 2.2).
169 First, we analysed the sensitivity of the NeQuick model on F10.7. Based on the results, we calculate a vector
170 $\mathbf{F10.7}(t)$ of the solar radio flux index with $\dim(\mathbf{F10.7}(t)) = 100 \times 1$ and $\mathbf{F10.7}(t) \sim N\left(\mathbf{F10.7}(t), \frac{3}{100}\right)$
171 $\mathbf{F10.7}(t)$ at time t . The vector $\mathbf{F10.7}$ serves as input for the NeQuick model to calculate the 100 ensembles of
172 X^b during the considered period and the initial guess of the electron densities $X^f(t_0)$.

173 An example on the variation of the generated ensembles is provided by **Figure 1**. ⁱⁿParticularly, we show in this
174 figure the distribution of the differences between the ensemble of electron densities $X^b(t)$ and the NeQuick model
175 values for DOYs 041 and 076. The residuals are depicted for a selected altitude and chosen UT times, presented
176 through different colors (cf. subfigure history). In addition, the mean, the standard deviation (STD) and the root
177 mean square (RMS) of the residuals are presented in the subplots.

- why this value?
- what is the impact at low SSAs?
If $F_{10.7} = 70$ then the std. dev. generated by this is only 2.1. This variation of $F_{10.7}$ in NeQuick would have very little impact.

This doesn't generate much variability in the ensemble. Do you envision this is a problem?

178 3 Validation scenario

179 Within this study, the EnKF with the different propagation methods is applied and validated for the tomography
180 of the topside ionosphere and plasmasphere. ~~Particularly,~~ Two periods with quiet (DOY 041-059, 2015) and
181 perturbed (DOY 074-079, 2015) ionospheric conditions are analysed. In this scope, we investigate the ability to
182 reproduce assimilated STEC as well as to estimate independent STEC measurements and in-situ electron density
183 measurements of the Swarm Langmuir Probes (LP).

184 In addition, we apply the tomography approach SMART+ (Gerzen and Minkwitz, 2016 and Gerzen et al., 2017)
185 to provide a benchmark. For SMART+ the number of iterations at each time step is set to 25 and the correlation
186 coefficients are chosen as described in Gerzen and Minkwitz (2016).

at least a couple of lines of description of SMART+ would be useful for the reader. Especially how the propagation works!

187 3.1 Reconstruction area

188 We estimate the electron density over the entire globe with a spatial resolution of 2.5 degrees in latitude and
189 longitude. Altitudes between 430 km and 20 200 km are reconstructed where the resolution equals 30 km for
190 altitudes from 430 km to 1000 km and decreases exponentially with increasing altitude for altitudes above 1000
191 km, i.e. in total 42 altitudes. Consequently, the number of unknowns is $K = 217728$. The temporal resolution is
192 set to 20 minutes.

193 3.2 Ionospheric conditions in the considered periods

194 We use the solar radio flux F10.7, the global planetary 3h index Kp and the geomagnetic disturbance storm time
195 (DST) index to characterize the ionospheric conditions during the periods of DOY 041-059 and DOY 074-079
196 2015. In the February period (DOY 041-059, 2015) the ionosphere is evaluated as quiet with F10.7 between 108
197 and 137 sfu, a Kp index below 6 and DST values between 20 and -60 nT. The 17-th of March (DOY 076) 2015 is
198 known as the St. Patrick's Day storm. The F10.7 value equals ~116 sfu on DOY 075 and ~113 sfu on DOY 076,
199 the Kp index is below 5 on DOY 075 and increases to 8 on DOY 076; DST drops down to -200nT on DOY 076.

How often above, e.g., 4? I wouldn't call that particularly quiet.



200 3.3 Data

201 3.3.1 STEC measurements

202 As input for the tomography approaches and for the validation, we use space-based calibrated STEC measurements
203 of the following satellite missions: COSMIC satellites, Swarm satellites, TerraSAR-X, MetOpA and MetOpB,
204 GRACE LEO satellites. Please note that in 2015, the orbit height of the COSMIC and MetOp satellites is ~800
205 km, the orbit height of the Swarm B and TerraSAR-X satellites is ~500 km and the one of the Swarm C satellite
206 ~460 km. The STEC measurements of Swarm A and GRACE are used only for the validation.

207 The STEC measurements of the Swarm satellites are acquired from <https://swarm-diss.eo.esa.int/> and the STEC
208 measurements of the other satellite missions are downloaded from <http://cdaac->
209 www.cosmic.ucar.edu/cdaac/tar/rest.html. Both data providers supply also information on the accuracy of the
210 STEC data. We utilize this information to fill the covariance matrix R of the measurement errors.

reference for each?

altitude for these?

accuracy?
or is it error?

211 3.3.2 In-situ electron density measurements from the Swarm Langmuir Probes

212 The LPs on board the Swarm satellites provide in-situ electron density measurements with a time resolution of 2
213 Hz. For the present study, the LP in-situ data are retrieved required from <https://swarm-diss.eo.esa.int/>. Further, information
214 on the pre-processing of the LP data is made available at the previous web address

215 Lomidze et. al (2018) assess the accuracy and reliability of the LP data (December 2013 to June 2016) by nearly
216 coincident measurements from low- and middle-latitude incoherent scatter radars, low-latitude ionosondes, and
217 COSMIC satellites, which cover all latitudes. The comparison results for each Swarm satellite are consistent across
218 these different measurement techniques. The results show that the Swarm LPs underestimate the electron density
219 systematically by about 10%.

220 4 Results

221 In this section, the different methods are presented with the following color code: blue for the method Rotation,
222 green for the method Exponential decay, light blue for the method Rotation with exponential decay, magenta for
223 NeQuick and red for SMART+. The legends in the figures are the following: “Rot” for the method Rotation, “Exp”
224 for the method Exponential decay, “Rot and Exp” for the method Rotation with exponential decay.



225 4.1 Reconstructed electron densities

226 At the end of each EnKF analysis step, we have, for each of the considered methods, 100 ensembles representing
227 the electron density values within the voxels. The EnKF reconstructed electron densities are then calculated as the
228 ensemble mean. The top subplots of **Figure 2** present the electron densities at DOY 076, 19:00 UT, reconstructed
229 by the method Rotation with exponential decay. The left hand side subplot shows horizontal layers of the topside
230 ionosphere at different heights between 490 and 827 km. The right hand side subplot shows the plasmasphere for
231 altitudes between 827 and 2400 km at chosen longitudes. The bottom line subplots show the vertical TEC maps
232 deduced from the 3D electron density in the considered altitude range between 430 and 20200 km for the same
233 time stamp. The left hand side subplot show the reconstructed values and the right hand side VTEC is deduced
234 from the NeQuick model calculated electron density. The reconstructed results are a bit higher than NeQuick ones.

can I check that
this plot has had
data assimilated
up to 1840 and then
propagated forward
by 20 mins
using the Rot+Exp
method?

some more description needed here.



235 **Figure 3** displays method Rotation reconstructed electron density layers at different heights between 490 and 827
236 km (left) and vertical TEC map deduced from the reconstructed 3D electron density in the altitude range between
237 430 and 20200 km (right) for the same DOY 076, at 19:00 UT. The method Rotation delivers much higher values
238 than NeQuick. All reconstructed values seems to be plausible, showing as expected the crest region, low electron
239 densities in the Polar regions, etc.

again, some more description of differences would help guide the reader. Alternatively you could plot the differences between the two methods.

240 4.2 Plausibility check by comparison with assimilated STEC

241 In this ^{Section} ~~chapter~~, we check the ability of the methods to reproduce the assimilated STEC measurements. For that
242 purpose, we calculate STEC along a ray path j , for all ray path geometries, using the estimated 3D electron
243 densities, denoted as $STEC_j^{est}$, and compare them with the measured STEC, $STEC_j^{meas}$, used for the
244 reconstruction. Then the mean deviation $\Delta STEC$ between the measurements $STEC_j^{meas}$ and the estimate $STEC_j^{est}$
245 is calculated for each of the considered methods according to

$$\Delta STEC(t_n) = \frac{1}{m} \sum_{j=1}^m (|STEC_j^{meas}(t_n) - STEC_j^{est}(t_n)|), \quad (13)$$

246 where m = number of assimilated measurements. $\Delta STEC$ is calculated at each epoch t_n . In terms of the notation
247 used for the Eqs. (1) - (4), we can reformulate the above formula for the mean deviation as

$$\Delta STEC(t_n) = \frac{1}{m} \sum_{j=1}^m (|y_j(t_n) - E(X_a(t_n))^T \cdot H_j|), \text{ with } H_j = j\text{-th row of } H. \quad (14)$$

move to separate line

248 Further, we consider the **RMS** of the deviations, in detail

$$RMS(t_n) = \sqrt{\frac{1}{m} \sum_{j=1}^m (|STEC_j^{meas}(t_n) - STEC_j^{est}(t_n)|)^2}. \quad (15)$$

249 To calculate $\Delta STEC$ and **RMS**, the same measurements are used as for the reconstruction. In this sense, the results
250 presented in **Figure 4 - Figure 8** can serve as a plausibility check, testing the ability of the methods to reproduce
251 the assimilated TEC.

252 **Figure 4** depicts the distribution of the residuals, left subfigure for the quiet period, right subfigure for the
253 perturbed period. The corresponding residual median, standard deviation (STD) and root mean square (RMS)
254 values are also presented in the figure. It is worth to mention here that during the quiet period, the measured STEC
255 is below 150 TECU. For all DOYs of the perturbed period, except DOY 076, the measured STEC is below ~130
256 TECU. On DOY 076, the STEC values rise up to 370 TECU.

257 The NeQuick model seems to underestimate the measured topside ionosphere and plasmasphere STEC during both
258 periods. During both periods, SMART+ seems to perform best, followed by the method Rotation. However, the
259 last one produces higher STD and RMS values. Compared to the NeQuick residuals, SMART+ is able to reduce
260 the median of the residuals by up to 86% during the perturbed and up to 79% during the quiet period. The RMS is
261 reduced by up to 48% and the STD by up to 41%. Rotation reduces the NeQuick median by up to 83%, the RMS
262 by up to 27%, the STD value is almost on the same level as for NeQuick. The method Exponential decay is able
263 to decrease the median of the NeQuick residuals by up to 54%, the RMS by up to 25%, and the STD values by up
264 to 13%. The method Rotation with exponential decay performs similar to the NeQuick model.

265 Interestingly, the median values are higher during the quiet period, while during the perturbed period the RMS and
266 STD values are significantly higher. The reason therefore is probably that the assimilated STEC values have in

Why does the method of time propagation have such an impact on the results? Wouldn't we expect the DA to dominate?

this seems surprising, I expected the method to do better. Perhaps more discussion needed as why this is.



267 average lower magnitude during the days in the perturbed period, compared to those during the quiet period (which
268 explains the lower median), except the storm DOY 076, while on DOY 076 they are significantly higher (which
269 explains the higher STD and RMS).

270 **Figure 5** and **Figure 6** plot $\Delta STEC$ values versus time for the selected periods. Noticeable is the increase of
271 $\Delta STEC$ during the storm on DOY 76. On the rest of the period, $\Delta STEC$ is below eight TECU. During both periods,
272 SMART+ generates the lowest $\Delta STEC$ values. $\Delta STEC$ of the methods Rotation and Exponential decay are in most
273 of the cases higher than SMART+ delta STEC values and lower than the NeQuick model. $\Delta STEC$ of the method
274 Rotation with exponential decay is similar to the NeQuick model.

275 **Figure 7** and **Figure 8** present the distribution of $\Delta STEC$ and the *RMS* error (cf. Eq. (14)) for the quiet and
276 perturbed periods respectively. **Figure 7** confirms the conclusions we draw so far from **Figure 4** and **Figure 5**.
277 SMART+ delivers the lowest $\Delta STEC$ and *RMS* values, followed by the method Rotation and then by the method
278 Exponential decay. Rotation with exponential decay performs similar to the NeQuick model. For the perturbed
279 period, again SMART+ delivers the lowest $\Delta STEC$ and *RMS* statistics, followed by the Exponential decay and
280 the Rotation with similar results.

281 4.3 Validation with independent space-based STEC data

282 In order to validate the methods with respect to their capability to estimate independent STEC, the LEO satellites
283 Swarm A and GRACE ^{have been used.} ~~are chosen.~~ The STEC measurements of these satellites are not assimilated by the tested
284 methods. It is to mention here that 2015 the Swarm A satellite was flying site on site with the Swarm C satellite at
285 around 460 km height. The height of the GRACE orbit was around 450 km. All satellites were flying ^{at} ~~on~~ almost
286 polar orbits.

I mentioned discussing this earlier.

287 For each of the ^{three} ~~two~~ LEOs, the residuals between $STEC^{meas}$ and $STEC^{est}$ are calculated and denoted as $dTEC =$
288 $STEC^{meas} - STEC^{est}$. Further, the absolute values of the residuals $|dTEC|$ are considered.

289 In general, for the quiet period, the STEC measurements of Swarm A vary below 105 TECU and for the second
290 period below 170 TECU. For the GRACE satellite, the STEC measurements are below 282 TECU for the quiet
291 period and below 264 TECU for the second period.

292 **Figure 9** and **Figure 10** display the histograms of the STEC residuals during the quiet period for Swarm A and
293 GRACE respectively. Presented are the distributions of the residuals $dTEC$ and the absolute residuals $|dTEC|$.
294 Also plotted are the median, STD and RMS of the corresponding residuals. **Figure 11** and **Figure 12** depict the
295 histograms of the STEC residuals during the perturbed period.

296 Again, the NeQuick model seems to underestimate the measured STEC during both periods for GRACE and
297 Swarm A satellites. Compared to the NeQuick model, during both periods, the methods SMART+ and Exponential
298 decay decrease the residuals and the absolute residuals between measured and estimated STEC for both GRACE
299 and Swarm A satellites. The method ^{Rotation} ~~with exponential decay~~ performs for both periods very similar to the
300 NeQuick model. The performance of the ^{Rotation} ~~with exponential decay~~ is partly even worse than the one of the background
301 model. Our impression is that the number and the distribution of the assimilated measurements is too small and
302 angle limited to be sufficient to dispense with a background model, as is the case with the Rotation method, which
303 uses the model only for the estimation of the systematic error.



304 Regarding the STEC of Swarm A, the lowest residuals and the most reduction in comparison to the NeQuick
305 model, are achieved by SMART+. The median and the STD of the SMART+ residuals are ~ 0.3 TECU and ~ 3.4
306 TECU ^{respectively} for quiet and ~ 0.7 TECU and ~ 7 TECU for the perturbed period. Compared to the NeQuick model,
307 the absolute median value is reduced up to 64% by SMART+ during the quiet and by up to 61% during the
308 perturbed period. The STD value is decreased by up to 47% during the quiet and up to 29% during the storm
309 period. The second lowest residuals are achieved by the Exponential decay - here the median of the residuals is
310 around 0.2 TECU for quiet and around 0.8 TECU for the perturbed period.

311 Regarding the STEC of GRACE during the quiet period, the lowest residuals and the most reduction in comparison
312 to background, are achieved by the Exponential decay, followed by SMART+. Exponential decay reduces the
313 background absolute median value by up to 26% and the STD value by up to 28%. The median of the residuals is
314 around 0.2 TECU. For SMART+, the median of the residuals is around 2.9 TECU. During the perturbed period,
315 SMART+ reduces the absolute median at most by 17% and the STD by 9%, the Exponential decay does not reduce
316 the absolute median, compared to NeQuick, but it reduces the absolute STD value by 23%. The median of the
317 residuals are around -0.5 TECU for Exponential decay and around 0.8 TECU for SMART+.

318 Comparing between quiet and storm conditions, in general an increase of RMS and STD of the residuals is
319 observable for the NeQuick model and all tomography methods regarding both satellites.

320 4.4 Validation with independent LP in-situ electron densities

321 In this section, we further ^{by what method?} extend our analyses to the validation of the methods with independent LP in-situ electron
322 densities of the three Swarm satellites. According to the locations of the LP measurements, the estimated electron
323 density values are interpolated from the 3D electron density reconstructions. For each satellite, the measured
324 electron density Ne^{meas} is compared to the estimated one Ne^{est} . In particular we calculate the residuals $dNe =$
325 $Ne^{meas} - Ne^{est}$, the absolute residuals $|dNe|$, the relative residuals $dNe_{rel} = \frac{dNe}{Ne^{meas}} \cdot 100\%$ and the absolute
326 relative residuals $|dNe_{rel}|$.

327 **Figure 13** depicts the distribution of the residuals dNe for the quiet period along with the median, STD and RMS
328 values. Each of the three subplots presents one of the Swarm satellites. In **Figure 14** the histograms of $|dNe|$ and
329 $|dNe_{rel}|$ are given for the same period. In **Figure 14** we do not separate the values for the different satellites,
330 because these are similar. **Figure 15** and **Figure 16** show the corresponding histograms for the perturbed period.

331 The electron densities of the NeQuick model are in median slightly higher than the LP in-situ measurements for
332 all three satellites during both periods. The median and STD values for the $|dNe_{rel}|$ residuals produced by
333 NeQuick are $\sim 33\%$ and $\sim 38\%$ resp. during the quiet period. For the perturbed period, we observe higher median
334 and STD values of $\sim 45\%$ and $\sim 56\%$, resp. The increase of the RMS and STD values of the absolute residuals is
335 also visible for all the considered reconstruction methods.

336 The methods SMART+ and Rotation with exponential decay follow the trend of the model and show similar
337 distributions in **Figure 13** and **Figure 15**. Comparing these two methods with the NeQuick model, the performance
338 of SMART+ is slightly better reducing the median of the absolute and absolute relative residuals by up to 8%.
339 Further, during both periods, SMART+ reduces the STD values of the $|dNe|$ values by up to 23%. However, the
340 STD and RMS values of the $|dNe_{rel}|$ residuals for SMART+ during the quiet period are higher than those of the
341 NeQuick model. The median and STD values of the $|dNe_{rel}|$ residuals for SMART+ are $\sim 30\%$ and $\sim 43\%$ resp.



342 during quiet and higher during perturbed period, namely ~43% and ~53% resp. The statistics of the methods
343 Exponential decay and Rotation are worse than those of NeQuick.

344 5 Summary and conclusions

345 In this paper, we focus on the assessment of three different propagation methods for an Ensemble Kalman Filter
346 approach in the case that a physical propagation model is not available or discarded due to computational burden.
347 We validate these methods with independent STEC observations of the satellites GRACE and Swarm A and with
348 independent Langmuir probes data of the three Swarm satellites. The methods are compared to the algebraic
349 reconstruction method SMART+, serving as a benchmark and to the NeQuick model for periods of the year 2015
350 covering quiet to perturbed ionospheric conditions. This work is carrying out our first case study in this regard.

351 Overlooking all the validation results, the methods SMART+ and Exponential decay reveal the best performance
352 with the lowest residuals. In general, the method Rotation with exponential decay follows the trends of the
353 NeQuick model. One significant difference between the investigated reconstruction approaches is that Rotation,
354 as the only one of considered methods, uses the background information only for the estimation of the systematic
355 error. The number of the assimilated measurements is small compared to the number of unknowns, additionally
356 the distribution of measurements is uneven and angle limited. We assume these are the main reasons, why the
357 method Rotation reproduces the assimilated STEC data well, but exhibits degraded results in comparisons with
358 independent data.

359 In summary, the comparison with the assimilated STEC show that during both periods all methods reduce
360 successfully the median, RMS and STD values of the STEC residuals in comparison to the background model.
361 SMART+ performs at best improving the statistics of the NeQuick model by up to 86%, followed by the method
362 Rotation, decreasing the median of the residuals by up to 83%. The method Exponential decay lowers the median
363 by up to 55%, but the STD values stay almost on the same level as for the NeQuick model.

364 Regarding the ability to estimate independent STEC measurements, the methods SMART+ and Exponential decay
365 reduce the independent STEC residuals by up to 64% for Swarm A and 28% for GRACE, compared to the NeQuick
366 model. SMART+ generates the smallest residuals for the STEC measurements of Swarm A and Exponential decay
367 performs at best for STEC measurements of GRACE.

368 Concerning the estimation of independent electron density data, SMART+ shows the best results, reducing the
369 background statistics of the absolute residuals by up to 23%. The median and STD values of the absolute residuals
370 $|dN_{e_{rel}}|$ for SMART+ are ~30% and ~43% resp. during quiet and higher, namely ~43% and ~53% resp. during
371 perturbed period. The distributions of the residuals produced by Rotation with exponential decay are similar to the
372 ones of the NeQuick model. In general, all the considered methods generate relatively high residuals. It should be
373 noted here that the independent electron density measurements are located at the lower edge of the reconstructed
374 area and all the assimilated measurements are located above. Additionally, as already mentioned in Section 3.3.2,
375 Swarm LPs was found to underestimate the true electron density systematically. This could be the second reason,
376 why the reconstructions, based on the STEC, do not match the LPs electron densities. To get better results for the
377 lower altitudes, it might be necessary to apply a kind of anchor point from below within the reconstruction
378 procedure. We plan to utilise therefor the Swarm LPs electron density measurements themselves.

But this is not one of the methods you are testing and could be significantly different in methodology to the other EnKF methods.

again a lot of this discussion talks about the skill and validity of SMART+. That is okay if you explicitly include SMART+ as one of the methods you want to test.



379 Further, to get a comprehensive concluding impression of the performance of the investigated methods and to get
380 an insight in the ability of the methods for correct characterization of the electron density profile shapes, we start
381 to work on comparisons with independent electron density data, located in the plasmasphere and with coherent
382 scatter radar data.

383 Furthermore, a pre-adjustment of the background model, e.g. in terms of F2 layer characteristics or the
384 plasmopause location, may be helpful to improve the reconstruction results (cf. e.g. Bidaine and Warnant, 2010,
385 Gerzen et. al., 2017).

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390 diss.esa.int/](https://swarm-diss.esa.int/)) and to the CDAAC: COSMIC Data Analysis and Archive Center for providing the STEC data of
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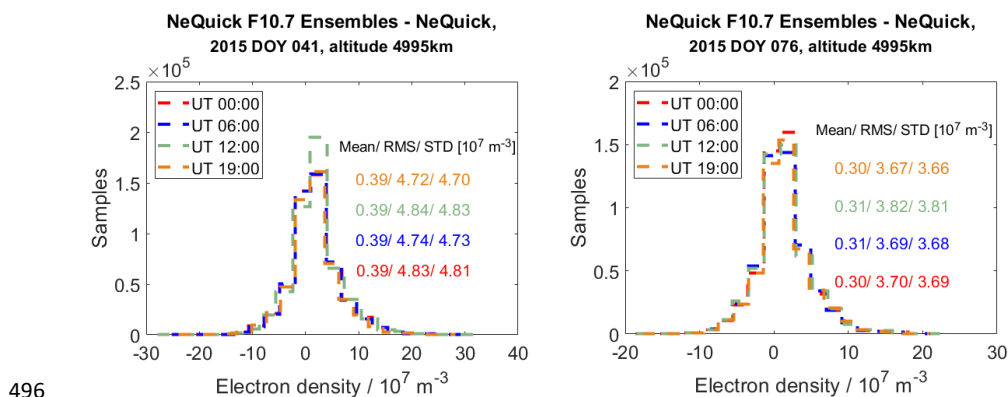
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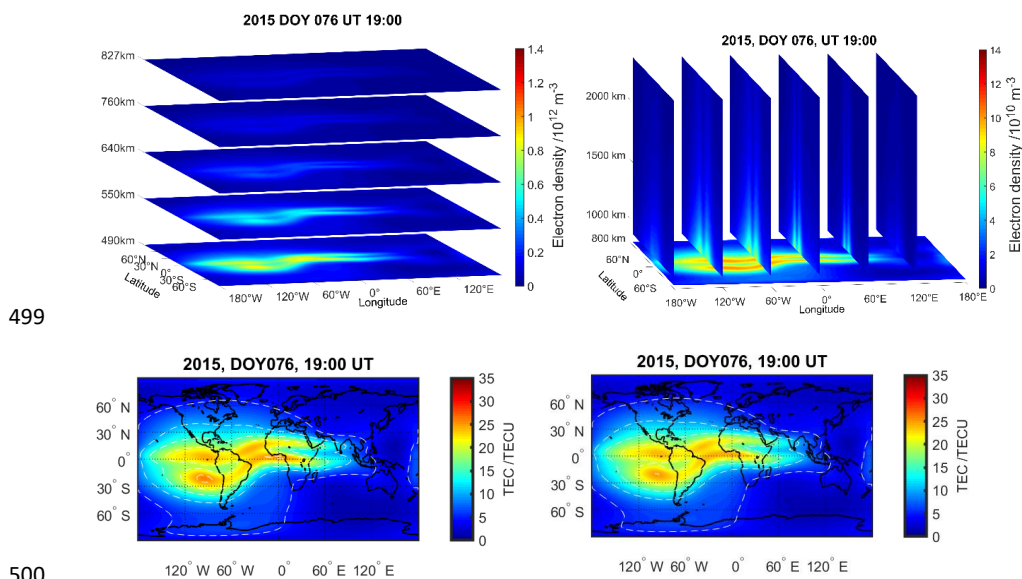
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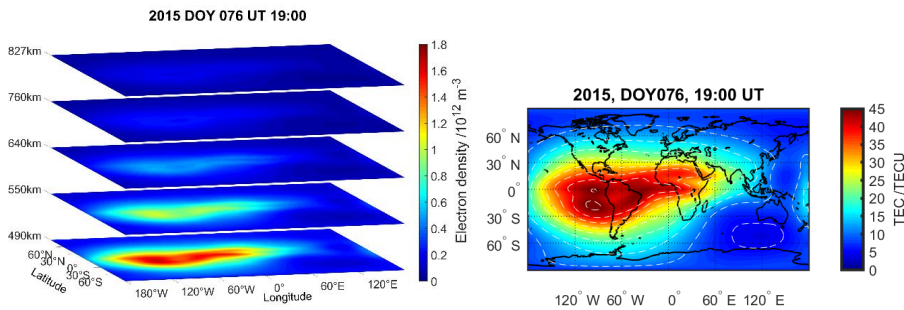
496
 497 **Figure 1: The distribution of the ensemble residuals for a chosen altitude and selected UT times, for all**
 498 **latitudes, longitudes. Left – for DOY 041, right – for DOY 076.**



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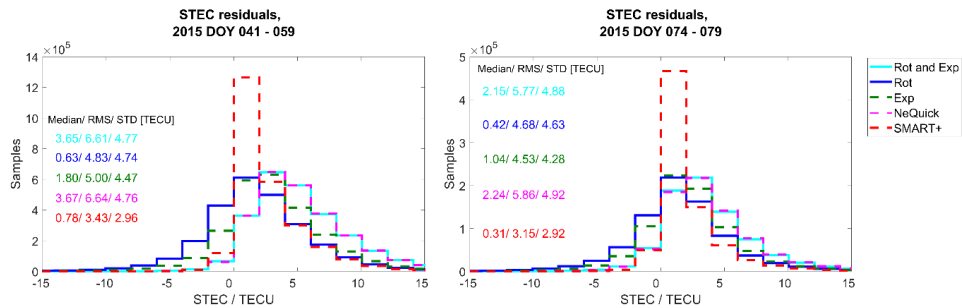


501 **Figure 2: Subfigures top: Rotation with exponential decay reconstructed electron density represented by**
 502 **layers at different heights between 490 and 827 km (left) and at chosen longitudes for altitudes between 827**
 503 **and 2400 km (right). Subfigures bottom: The vertical TEC map deduced from the reconstructed (left) and**
 504 **NeQuick-modeled (right) 3D electron density in the altitude range between 450 and 20200 km.**



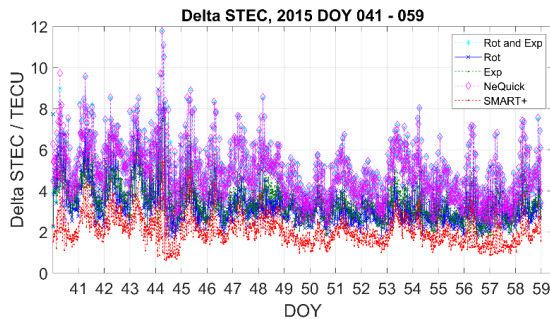
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506 **Figure 3: Subfigures top: Method Rotation reconstructed electron density represented by layers at different**
 507 **heights between 490 and 827 km (left) and vertical TEC map deduced from the reconstructed 3D electron**
 508 **density in the altitude range between 450 and 20200 km (right).**



509

510 **Figure 4: Plausibility check – distributions of the STEC measured – STEC estimated residuals. Left**
 511 **subfigure depicts residuals of the quiet period, right subfigure for the perturbed period.**

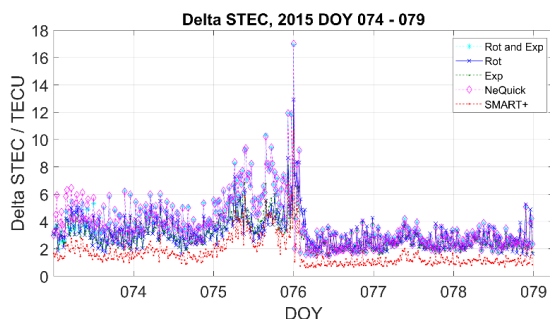


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513 **Figure 5: Plausibility check for the quiet period – Δ STEC values versus time.**

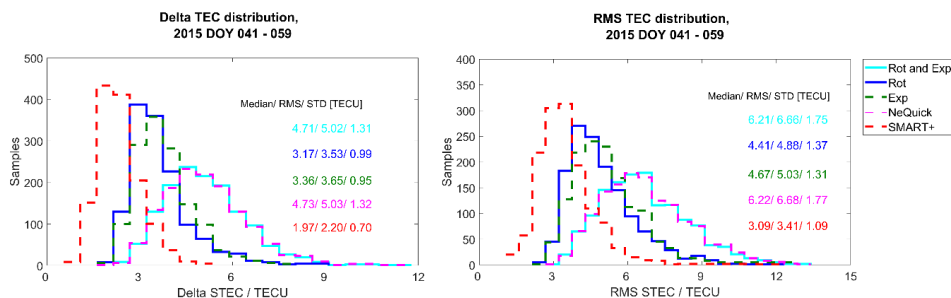
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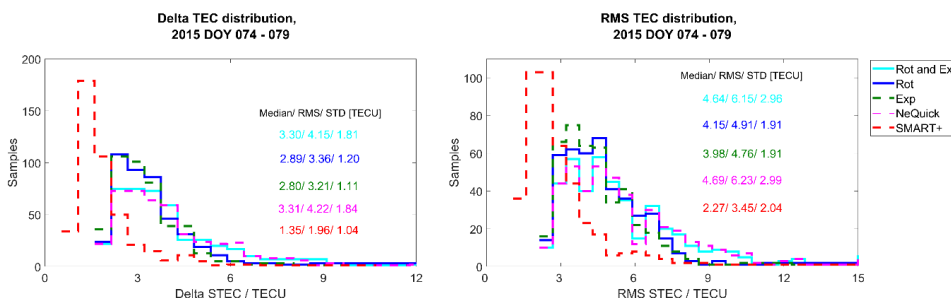
516

517 **Figure 6: Plausibility check for the perturbed period – Δ STEC values versus time.**



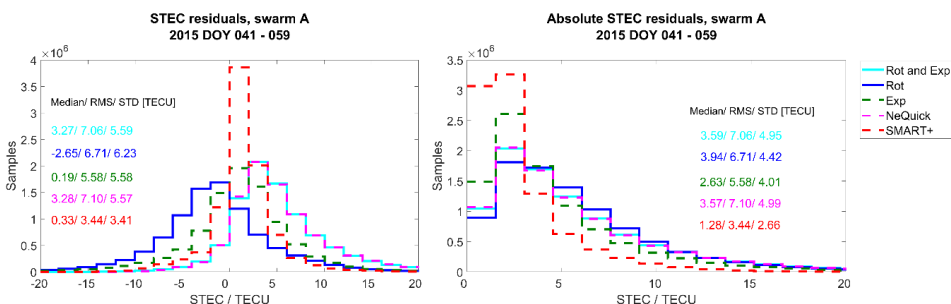
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519 **Figure 7: Plausibility check for the quiet period – distributions of the delta TEC (left) and RMS (right)**
 520 **values.**



521

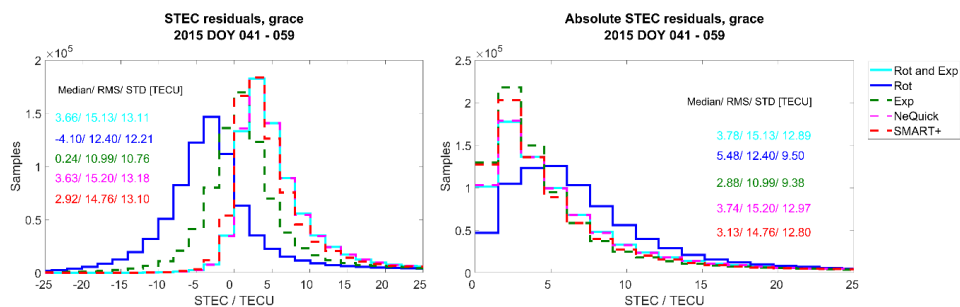
522 **Figure 8: Plausibility check for the perturbed period – distributions of the delta TEC (left) and RMS (right)**
 523 **values.**



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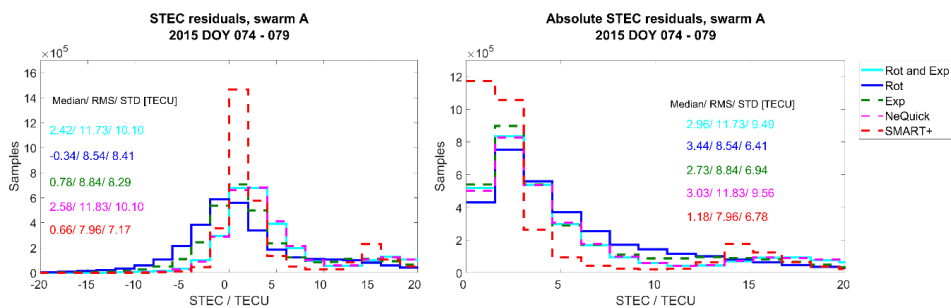


525 **Figure 9: Histograms of the STEC residuals (left) and absolute residuals (right) during the quiet period, for**
 526 **Swarm A.**



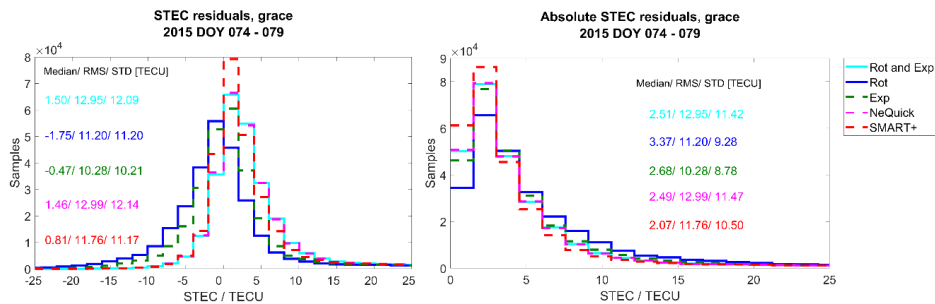
527

528 **Figure 10: Histograms of the STEC residuals (left) and absolute residuals (right) during the quiet period,**
 529 **for GRACE.**



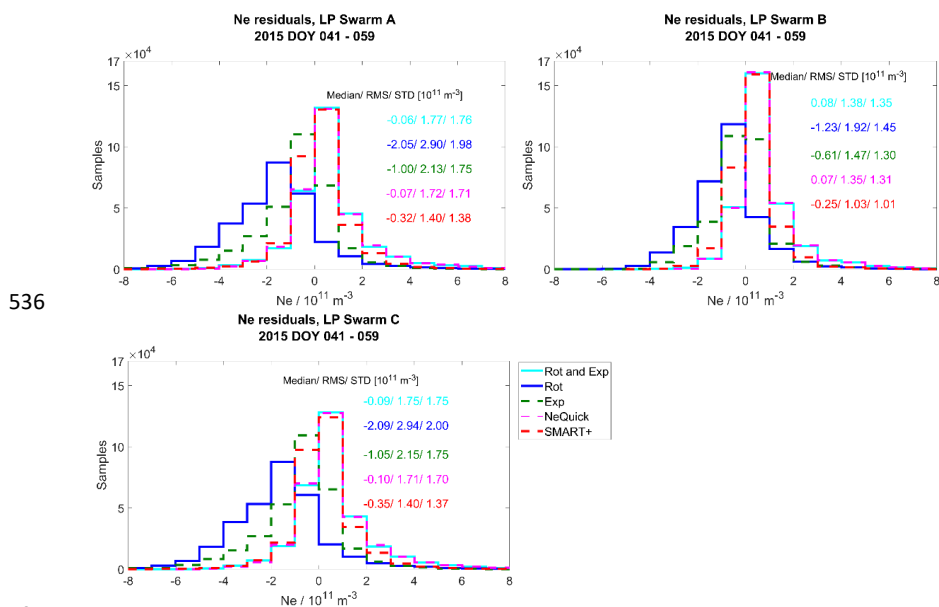
530

531 **Figure 11: Histograms of the STEC residuals (left) and absolute residuals (right) during the perturbed**
 532 **period, for Swarm A.**

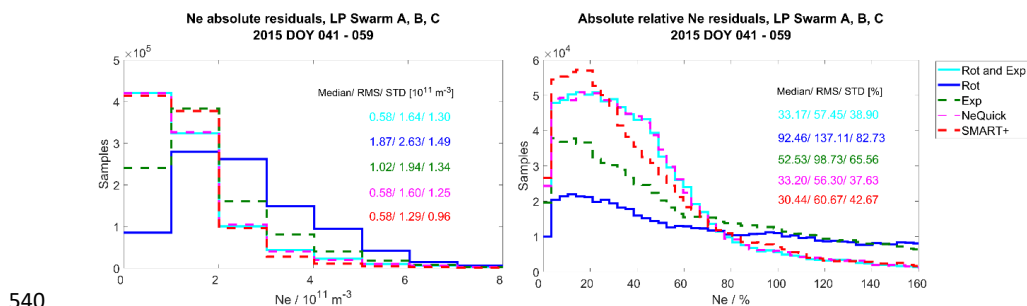


533

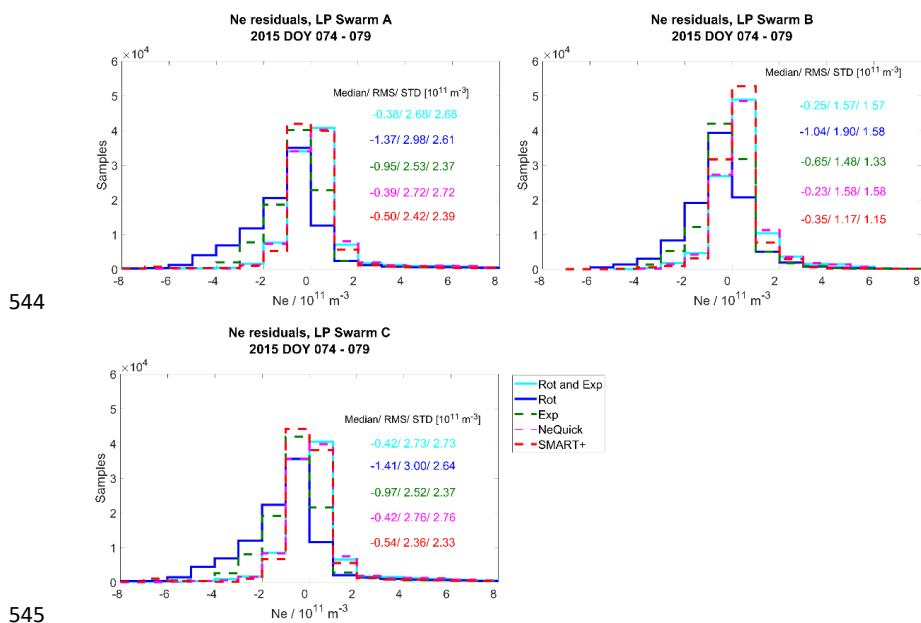
534 **Figure 12: Histograms of the STEC residuals (left) and absolute residuals (right) during the perturbed**
 535 **period, for GRACE.**



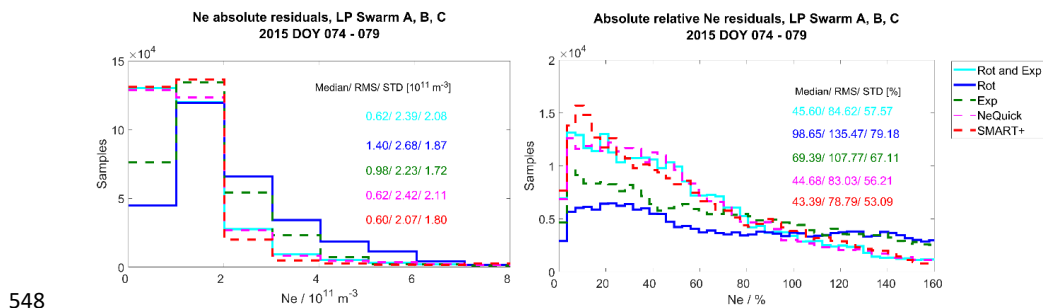
538 **Figure 13: Validation with LP data – distribution of the Swarm A, B, C (separated) electron density**
 539 **residuals for the quiet period.**



542 **Figure 14: Validation with LP data – distribution of the Swarm absolute and absolute relative electron**
 543 **density residuals for the quiet period.**



546 **Figure 15: Validation with LP data – distribution of the Swarm A, B, C (separated) electron density**
 547 **residuals for the perturbed period.**



549 **Figure 16: Validation with LP data – distribution of the Swarm absolute and absolute relative electron**
 550 **density residuals for the perturbed period.**