

EMPIRICAL MODELLING OF ION TRANSITION LEVELS BASED ON SATELLITE IN-SITU MEASUREMENTS

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Abstract

The mathematical formulation of a new empirical model of $O^+ - H^+$ and $O^+ - He^+$ transition levels is presented. The model is based on ion composition measurements carried out onboard satellites like the Atmosphere Explorer, Dynamics Explorer, Orbiting Geophysical Observatory, etc. The modelling approach offers opportunities for strict control on data acquisition and processing, convenient approximation when referencing the levels, and multiple research applications.

Key words: ion transition levels, empirical modelling, satellite measurements

Introduction. The $X^+ - Y^+$ ion transition height (level) is defined [1] as the height where the ion gas is composed of equal parts of two ion species X^+ and Y^+ ; below this height X^+ dominates over Y^+ , above the height Y^+ dominates over X^+ . There are several ion transition levels of interest, $O^+ - H^+$, $O^+ - He^+$, $NO^+ - O^+$, etc., which are important characteristics of the ionosphere and plasmasphere. The transition height studies can deepen our insight into various underlying chemical and transport processes, ionospheric storms, ion composition [1-3], etc. These levels may also serve as reference points when developing ionospheric and plasmaspheric models [4].

This paper presents the mathematical formulation of a new model of $O^+ - H^+$ and $O^+ - He^+$ transition levels based on satellite in-situ measurements of the individual ion densities.

Geophysical parameters. The first step in developing the model is the definition of model input parameters. The transition levels manifest substantial variability at different spatial and temporal conditions. Considering previous plasma composition studies [1-3], the required set of model parameters is: solar activity, season, local time, geomagnetic longitude, and geomagnetic latitude. It is important to arrange a proper discretisation with respect to each parameter in order to cover the characteristic trends in its values and also to secure sufficient amount of data within a discretisation interval.

Data acquisition and processing. The most reliable source of information about the ion transition levels is the satellite in-situ measurement technology; the data acquisition is based on measurements of the individual ion concentrations at altitudes where the transition occurs. Two methods, 'direct' and 'profile', are proposed here to derive the $X^+ - Y^+$ transition height from X^+ and Y^+ ion concentrations. Adopting

a spherical coordinate system originating from the Earth's centre, the concentration of the i -th ion species at a given moment and space point is $n_i = n_i(r, \theta, \varphi)$, where the space coordinates of the point are: r – radial distance, θ – colatitude, and φ – longitude. The distance $\delta(i, j)$ between two instances of measurement, $n_i(r, \theta, \varphi)$ and $n_j(r + dr, \theta + d\theta, \varphi + d\varphi)$, is defined as $\delta(i, j) = (dr^2 + r^2.d\theta^2 + r^2 \sin^2 \theta.d\varphi^2)^{1/2}$ and the relative density difference is $\rho(i, j) = |n_i - n_j| / \max(n_i, n_j)$.

The 'direct' method records all values of the radial distance (i.e. height) r , for $\delta(i, j) \leq \varepsilon_{\text{space}}$ and $\rho(i, j) \leq \varepsilon_{\text{dens}}$. A 'perfect' TL encounter, i.e. $\varepsilon_{\text{space}} = 0$ and $\varepsilon_{\text{dens}} = 0$, is observed rarely and is of little practical help. Therefore, the error tolerances, $\varepsilon_{\text{space}}$ and $\varepsilon_{\text{dens}}$, are set to optimal positive values, small enough to secure statistically significant data acquisition. The main advantage of the 'direct' method is in the high accuracy it provides when data are in abundance.

The 'profile' method deduces the transition level from the altitude density distribution (profile) of the individual ions – the transition level being the height where the ion profiles intersect. Each profile is obtained after averaging (over height) of the ion concentration measurements binned into a latitude-longitude rectangle. The main advantage of the method is in the opportunity for reliably interpolating (extrapolating) the ion profiles and consequently deducing the level in many cases where the 'direct' method fails to record the transition level.

Data base construction. A standard approach to revealing the behaviour of a given parameter is to fix the rest of the parameters and to fit the collected data with a convenient function if necessary. However, the spatial variations are treated in a slightly different manner than the temporal variations.

Fourier analysis is a valuable instrument in the investigation of the temporal (solar activity, diurnal and annual) variations because it provides easy access to the study of data periodicities. Another advantage is that a given set of time domain data is transformed into a fixed (limited) number of Fourier series coefficients. This can be done in the following manner. For a given spatial location and solar activity, the diurnal course of the transition level, presented as a function of the local time and month, is

$$(1) \quad f(t, m) = a_0(m) + \sum_{i=1}^{n_{\max}} a_i(m) \cos\left(i \frac{2\pi}{T} t\right) + \sum_{i=1}^{n_{\max}} b_i(m) \sin\left(i \frac{2\pi}{T} t\right),$$

where t is the local time, T is the period ($T = 24$ if the dimension of t is hour), m is the number of the month, and n_{\max} is the number of the harmonic with the highest frequency. The criterion employed for identifying n_{\max} is – the half-period of the highest-frequency harmonic should be larger than the length of the biggest data gap. The TL annual variations are expressed by a spectral decomposition of the coefficients describing the diurnal variation. It is important to note that the discrete Fourier expansion is equivalent to the discrete Fourier transform of a finite time series. Due to linearity of the Fourier transform, it makes no difference which variation is analysed first – the annual or the diurnal variation. However, the above linearity is not preserved when amplitudes and phases are used instead of cosine and sine coefficients.

When constructing the data base in terms of the spatial variations, the application of the above-described 'direct' and 'profile' acquisition methods leads to some discrepancies between the corresponding values obtained by both methods; the average value and the amplitude of the variation are mostly affected. The differences are due mainly to the following factors, [4]: limited number of measurements in some temporal and/or spatial intervals, inaccuracies in the extrapolation of ion density profiles, the error tolerance allowed when obtaining the direct encounters, etc. The following reconciliation approach is offered, demonstrated on the longitudinal variations which are most seriously affected. The aim is to obtain the value y_{ij} of the transition level at

its corresponding set point (i, j) by using both average density profiles and TL direct measurements data. The idea is to start from the value a_j (the transition level deduced from the density profile for a given j -th latitude band) and to 'distribute' this value over the whole longitude range 0 – 360° while preserving the longitudinal behaviour pattern obtained by both methods. The following 'distribution' formula is constructed:

$$(2) \quad y_{ij} = \{\alpha_j a_j + (1 - \alpha_j) \cdot [\beta_j x_{mj}^{(p)} + (1 - \beta_j) x_{mj}^{(d)}]\} \cdot \{1 + \beta_j \chi_j^{(p)} + (1 - \beta_j) \chi_j^{(d)}\},$$

where $i = 1, 2, \dots, n_i$, $j = 1, 2, \dots, n_j$, and also

$$\chi_j^{(*)} = (x_{ij}^{(*)} - x_{mj}^{(*)}) / x_{mj}^{(*)}, \quad x_{mj}^{(*)} = \frac{1}{n_i} \sum_{i=1}^{n_i} x_{ij}^{(*)}, \quad j = 1, 2, \dots, n_j.$$

The value x_{ij} is the transition level at a mesh point (i, j) obtained from 'direct measurement' (superscript (d)) and 'profile' (superscript (p)), respectively; the mean value for a given j -th latitude band is denoted by x_{mj} . The weights α and β vary in the interval $[0, 1]$ and the most important criteria on determining these coefficients are the data number and scattering. The weight β exists to reconcile the different ways of deducing the level – direct and profile: if a 'direct' value is found to be more reliable, the weight β should be set close to 0; if a 'profile' value is more reliable, β should be set close to 1. The discrepancies observed between the transition level's values deduced from averaged ion density profiles and the values directly encountered by the satellite are attributed mostly to the following factors: nature of the averaging process in altitude direction, the inevitable density tolerance (no matter how small it is) used for data processing may lead to errors especially when the proximity of O^+ and He^+ density values lasts for an extended height interval, existence of data gaps in the altitude distribution of the ion densities, limited data in some temporal and spatial intervals, etc. The other weight α is used to minimise possible extrapolation errors when deducing values by the 'average profile' method.

Approximation. In order to provide easy access to values between the grid points, the transition level is approximated by the following multi-variable polynomial:

$$\begin{aligned} P(C, N; X) &= \sum_I C(I) \cdot G(I, X) \\ &= \sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} \sum_{i_3=1}^{n_3} \sum_{i_4=1}^{n_4} \sum_{i_5=1}^{n_5} C(i_1, i_2, \dots, i_5) \cdot g_1(i_1, x_1) \cdot g_2(i_2, x_2) \dots g_5(i_5, x_5), \end{aligned}$$

where

$$\begin{aligned} C(I) &= C(i_1, i_2, \dots, i_5) && \text{—coefficients} \\ G(I, X) &= g_1(i_1, x_1) \cdot g_2(i_2, x_2) \dots g_5(i_5, x_5) && \text{—generalised basis function} \\ N &= (n_1, n_2, \dots, n_5) && \text{—number of basis functions} \\ I &= (i_1, i_2, \dots, i_5), \quad i_m = 1, 2, \dots, n_m; \quad m = 1, 2, \dots, 5 && \text{—indices} \\ X &= \prod_{m=1}^5 [x_L^{(m)}, x_R^{(m)}], \quad x \in X \subset \mathbb{R}^5 && \text{—variables} \end{aligned}$$

The set $\{g_m(i_m, x_m)\}_{i_m=1}^{n_m}$ is a system of linearly independent functions on the domain of the m -th parameter. Particularly convenient orthogonal systems are, [5]: algebraic basis $(1, x, x^2, \dots, x^{n_m})$, trigonometric basis $(1, \sin x, \cos x, \dots, \sin n_m x, \cos n_m x)$;

Chebyshev basis ($\cos(n \arccos x)$, $n = 1, 2, \dots, n_m$). The choice depends mainly on the type of variations induced by a particular geophysical parameter. The use of algebraic polynomials is the easiest way of approximating all types of the level variations securing high accuracy near the data points. The trigonometric approximation [6] is very useful when approximating a periodic function; the set is orthogonal over any interval and the derivative of each member is also a member. The Chebyshev polynomials [7] are orthogonal in the interval $[-1, 1]$ over a weight $(1 - x^2)^{-1/2}$, and the approximation using these polynomials provides the smallest maximum deviation from the 'true' function.

Numerical method for calculating the approximation coefficients. The method of least squares fit is applied for calculating the fitting coefficients. The model's data base is denoted by $\{x_n, y_n, p_n\}_{n=1}^{ND}$ where $x_n = (x_{n1}, x_{n2}, \dots, x_{n5})$ is a data point ($x_n \in \mathfrak{R}^5$), y_n is the value at x_n ($y_n \in \mathfrak{R}^1$), p_n is the weight, ND is the number of data points. A set of coefficients $\{C(I)\}_I$ is being sought, for which the functional

$$F(C) = \left\{ \sum_{n=1}^{ND} p_n (y_n - P(C, N; X))^2 \right\}^{\frac{1}{2}}$$

reaches its minimum. That means the following system should be solved:

$$\frac{dF}{dC_I} = 0, \quad I \in \mathbb{N}^5, \quad I \leq N$$

that is (in matrix form)

$$A(I, J).C(I) = B(I),$$

where

$$A(I, J) = \sum_{n=1}^{ND} p_n G(I, x_n).G(J, x_n), \quad B(I) = \sum_{n=1}^{ND} p_n G(I, x_n)y_n,$$

$$I \in \mathbb{N}^5, \quad I \leq N, \quad 1 \leq i_m \leq n_m, \quad J \in \mathbb{N}^5, \quad J \leq N, \quad 1 \leq j_m \leq n_m.$$

The numerical solution of the above system of equations delivers the required coefficients $C(I)$.

Results and discussion. The model has been tested extensively for various spatial and geophysical conditions. A very good measurement database for developing and testing purposes offers the AE-C (Atmosphere Explorer-C) satellite. The satellite was launched on 13/12/1973 in an elliptical orbit (inclination 68.1°) collecting a large database of ionospheric and thermospheric densities, temperatures, winds, and emissions within the altitude range of 130–4300 km.

The O^+ , H^+ , and He^+ ion concentrations used in this study are obtained during the first 16 months of the mission, from 16/12/1973 to 21/3/1975, when the solar activity was low. Measurements from both the Bennett and Magnetic ion-mass spectrometers have been utilized.

In order to obtain a general idea of the models performance, the diurnal behaviour of $O^+ - H^+$ and $O^+ - He^+$ transition levels are compared with actual AE-C measurements (Fig. 1) for equinox conditions. For the purpose of comparison, data from all longitudes and within the $(-60^\circ; +60^\circ)$ geomagnetic latitude band are collected during the vernal and autumn equinoxes (defined as 91-day periods centred on the equinoxes). The direct encounters of the levels are obtained with density tolerance of $\varepsilon_{\text{dens}} = 0.01$ height

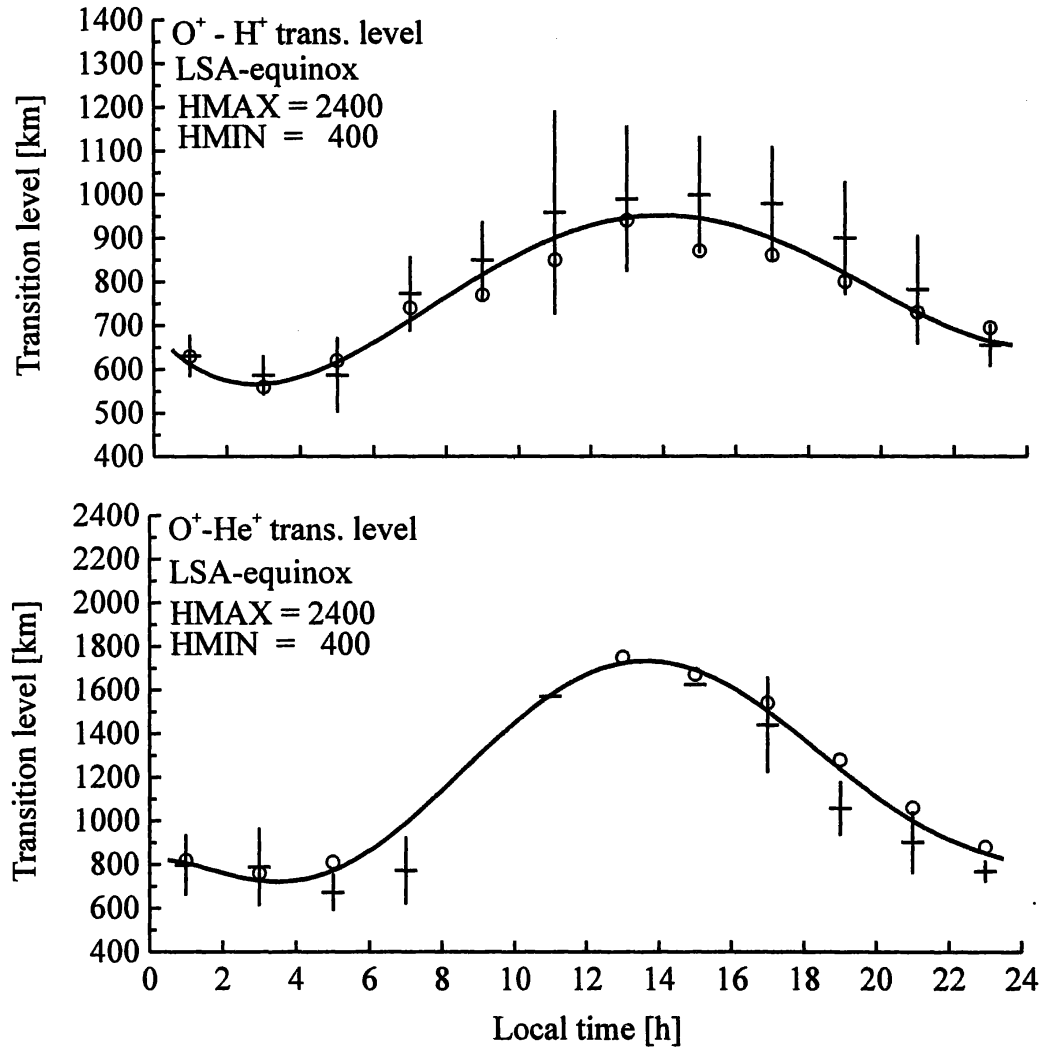


Fig. 1. Diurnal variations of $O^+ - H^+$ (top panel) and $O^+ - He^+$ (bottom panel) transition levels as measured by AE-C satellite. HMIN and HMAX indicate the height limits over which the data were taken. Direct encounters are obtained with density tolerance $\varepsilon_{\text{dens}} = 0.01$; the averages are denoted with horizontal bars, standard deviations with vertical bars, the open circles indicate the values deduced from averaged ion density profiles. The solid line represents the model calculations

tolerance of 1 km, latitude and longitude tolerances of 1 degree. The profile method uses individual ion densities averaged over 20 km in altitude. The model calculations are carried out for the spatial and temporal conditions closely matching those during the satellite mission; the results from different latitudes (10° -wide step) are averaged. In terms of overall performance, the developed transition level models perform quite well particularly for low solar activity conditions. The simulated values are well within the natural variations of the measurement data. The effect of using the distribution formula (2) is clearly seen in Fig. 1 showing that the model results are between the 'direct' and 'profile' acquisition method values.

Conclusions. The mathematical formulation of a new $O^+ - H^+$ and $O^+ - He^+$ transition height model has been presented. The modelling approach is reliable since it is based on the most reliable source for obtaining the transition levels – in-situ satellite

and rocket measurements. In addition, the proposed data acquisition and processing method provides opportunity for strict and unified statistical control on retrieving the transition levels. Another advantage of the technique is its flexibility: the model provides convenience when referencing the level with respect to the most important geophysical parameters; the model can be easily upgraded when more data become available; models of other transition levels could be developed using the same technique. Many applications are envisaged: development and evaluation of empirical and theoretical ionosphere/plasmasphere models, reconstruction of the vertical electron density structure using TEC measurements [8], etc.

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