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Atmospheric ionization induced by precipitating electrons: Comparison of CRAC:EPII model with a parametrization model

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ABSTRACT

Results of a comparison of a new model CRAC:EPII (Cosmic Ray Atmospheric Cascade: Electron Precipitation Induced Ionization) with a commonly used parametric model of atmospheric ionization is presented. The CRAC:EPII is based on a Monte Carlo simulation of precipitating electrons propagation and interaction with matter in the Earth's atmosphere. It explicitly considers energy deposit: ionization, pair production, Compton scattering, generation of Bremsstrahlung high energy photons, photo-ionization and annihilation of positrons, multiple scattering as physical processes accordingly. Propagation of precipitating electrons and their interactions with air is simulated with the GEANT4 simulation tool PLANETOCOSMICS code using NRLMSISE-00 atmospheric model. Ionization yields are computed and compared with a parametrization model for different energies of incident precipitating energetic electrons, using simulated fluxes of mono-energetic particles. A good agreement between the two models is achieved in the mesosphere but the contribution of Bremsstrahlung in the stratosphere, which is not accounted for in the parametric models, is found significant. As an example, we calculated profiles of the ion production rates in the middle and upper atmosphere (below 100 km) on the basis of balloon-born measured spectra of precipitating electrons for 30-October-2002 and 07-January-2004.

1. Introduction

The main source of ionization in the troposphere and stratosphere is due to cosmic rays (O'Brien, 1970; Usoskin and Kovaltsov, 2006; Bazilevskaya et al., 2008; Stozhkov et al., 2009; Velinov et al., 2013; Mironova et al., 2015), which are mostly protons and α-particles originating from outer space (Gaisser and Stanev, 2010). In addition to energetic CR particles, a softer electron component of corpuscular radiation is present in the near-Earth space, that ionizes the atmosphere and specifically its upper part (see Li and Temerin, 2001, and references therein). Precipitation of electrons into the atmosphere occurs from various regions of the magnetosphere resulting from different mechanisms, some of them are still poorly understood (e.g. Dorman, 2004; Mironova et al., 2015, and references therein). Precipitating electrons play an important role in ion production in the Earth's atmosphere, specifically over polar regions (Makhmutov et al., 2003a; Daae et al., 2012; Clilverd et al., 2013). They affect the atmospheric chemistry (e.g. Rozanov et al., 2005; Verronen et al., 2011; Daae et al., 2012; Mironova et al., 2015) as well as physical properties of the atmosphere and magnetosphere (e.g. Makhmutov et al., 2003a; Clilverd et al., 2008; Maliniemi et al., 2013). The intensity of electron precipitation depends on solar activity (Neal et al., 2015; Makhmutov et al., 2001), season (Makhmutov et al., 2003b), geomagnetic activity (Park et al., 2013; Rodger et al., 2007; Horne et al., 2009) and other factors (Makhmutov et al., 2006). Therefore, a convenient model for assessment of the atmospheric ionization due to precipitating electrons would stimulate better understanding of the impact of energetic particle on atmospheric processes (e.g. Mironova et al., 2015, and references therein).

Interactions between precipitating electrons and the atmosphere can be modelled in different ways, for example by solving Boltzman transport equations (O'Brien, 1970; Frahm et al., 1997), parameterized using approximations (e.g. Fang et al., 2008, 2010; McGranaghan et al., 2015) or directly simulated by a Monte Carlo method (Solomon, 1993; Wissing and Kallenrode, 2009; Wissing et al., 2011). Here we consider a recent parametrization model based on earlier developed multi-stream and first-principle models (see Fang et al., 2008, and references therein). The background atmosphere for this model is from MSIS-family models (Picone et al., 2002). These models effectively include earlier models of the same family (e.g., Lummerzheim et al., 1989;

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Lummerzheim and Lilensten, 1994), therefore we focus here only on the recent model by Fang et al. (2010).

Although direct ionization is straightforward to be included into a parameterization model, one important process, viz. Bremsstrahlung, which contributes to atmospheric ionization at lower and middle altitudes (Frahm et al., 1997) is not intrinsically there. Accordingly, the parametrization model is well validated for the upper atmosphere, but it could lead to some uncertainties in the middle and lower atmosphere because of that. Here we check the role of this process in the ionization modelling. On the other hand, Monte Carlo approach includes realistically all the known physics processes involved. Such models are usually based on the response (yield) function formalism, using precomputed ionization yields. This approach allows more precise results, especially for the high energy range and lower atmosphere, because of off-line computation with high statistics and simulation of mono-energetic particles (e.g. Usoskin and Kovaltsov, 2006; Velinov et al., 2013; Mishev and Velinov, 2014).

The use of the off-line calculated yield function with high precision is flexible for a user as it only requires a simple integration of a product of the independently known spectrum of electrons with the yield function.

In this work, we compare a new Monte Carlo model of the CRAC family for assessment of atmospheric ionization due to precipitating electrons and compare it with a previously proposed parametrization model. The general aim of this work is a quantitative comparison and validation of our model to estimate the electron impact ionization. The new family-CRAC model, whose detailed description is given elsewhere (Artamonov et al., 2016), is an extension of the CRAC model for CR induced ionization (Usoskin and Kovaltsov, 2006; Usoskin et al., 2010), based on the ionization yield function formalism. It is a full target model similar to CRAC model for cosmic ray induced ionization and other similar models based on a Monte Carlo simulation of the atmospheric cascade (e.g. Desorgher et al., 2005; Usoskin and Kovaltsov, 2006; Velinov et al., 2009).

2. The model CRAC:EPII

Monte Carlo simulations possess an advantage compared to parameterization models by considering realistically all the physics processes involved. It requires heavy numerical computations, which were done once with a cluster computer. The results were summarized in look-up tables (Artamonov et al., 2016) which make it easy for practical use in other codes.

Here we apply Monte Carlo simulations of electron propagation and interaction with matter in the Earth's atmosphere. The main advantage of Monte Carlo transport codes is that they consider, in a realistic manner, physics processes, namely energy deposit, ionization, pair production, Compton scattering, generation of Bremsstrahlung high energy photons, photo-ionization and annihilation of positrons. Moreover the multiple scattering of electrons is also realistically considered. In addition, since electrons produce Bremsstrahlung photons which penetrate deeper in the atmosphere, compared to primary particles (e.g. Schrøter et al., 2006), and produce ionization there, it is important to use adequate modelling of their production and propagation.

In this work propagation of precipitating electrons and their interactions with air, leading to production of secondary particles, is modelled using the GEANT4 based (Agostinelli et al., 2003) simulation tool PLANETOCOSMICS (Desorgher et al., 2005). Here we use a realistic curved atmospheric model NRLMSISE-00 (Picone et al., 2002). The code represents a Monte Carlo simulation tool for detailed study of cascade evolution in the atmosphere initiated by various primary particles including electrons. The PLANETOCOSMICS allows simulation of a purely electromagnetic cascade in a realistic manner.

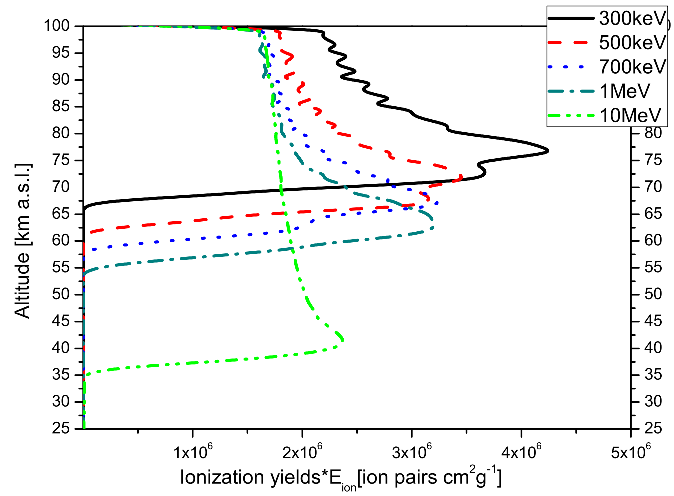

Fig. 1. Ionization yields for primary electrons with given energy as a function of the altitude above the sea level, computed with CRAC:EPII model.

We have computed, with high statistics, the ionization yields (response function) i.e. the number of ion pairs produced per gram of ambient air at a given atmospheric depth by a single primary precipitating electron with a given energy. The computations were carried out for energetic electrons in the energy range between 50 keV and 500 MeV. An example of ionization yields for several energies of primary electron is given in Fig. 1.

The ionization yield Y, given in units of ion pairs cm^2 g^{-1}, at the atmospheric depth x, is defined as:

$$Y(x, K) = \frac{\Delta E}{E_i \Delta x} \qquad (1)$$

where ΔE is the mean energy deposit in the atmospheric layer Δx centred at the atmospheric depth x per one simulated primary electron with the kinetic energy K, and E_i=35 eV is the average energy needed to produce one ion pair in air (Porter et al., 1976).

The ionization yield $Y(x, K)$ is related to the ion production rate $Q(x)$ at a given depth x as:

$$Q(x) = \int_{E_i}^{\infty} \frac{dJ_e}{dK} Y(x, K)\rho(x)dK \qquad (2)$$

where $\frac{dJ_e}{dK}$ is the differential energy spectrum of the primary precipitating electrons with kinetic energy K, $\rho(x)$ is the atmospheric density at given atmospheric depth x. As expected, the maximum of ionization yields strongly depends on the energy of the precipitating electron. The maximum is located lower for electrons with greater energy (Fig. 1). In addition, significant fluctuations, specifically in a low energy range, of ionization yields are observed at altitudes of about 90 km. They are due to intrinsic fluctuations of atmospheric cascades which are not developed of that altitude, rather than an insufficient number of test particles in the model run.

3. Comparison with a parametrization model

There are several parametrization models for assessment of electron induced ion production in the atmosphere (e.g. Lazarev, 1967; Roble and Ridley, 1987; Frahm et al., 1997; Fang et al., 2010). Some of the models were focused on evaluation of auroral electron impact ionization (e.g. Roble and Ridley, 1987). In order to assess production of NO_x in the middle and upper atmosphere by high

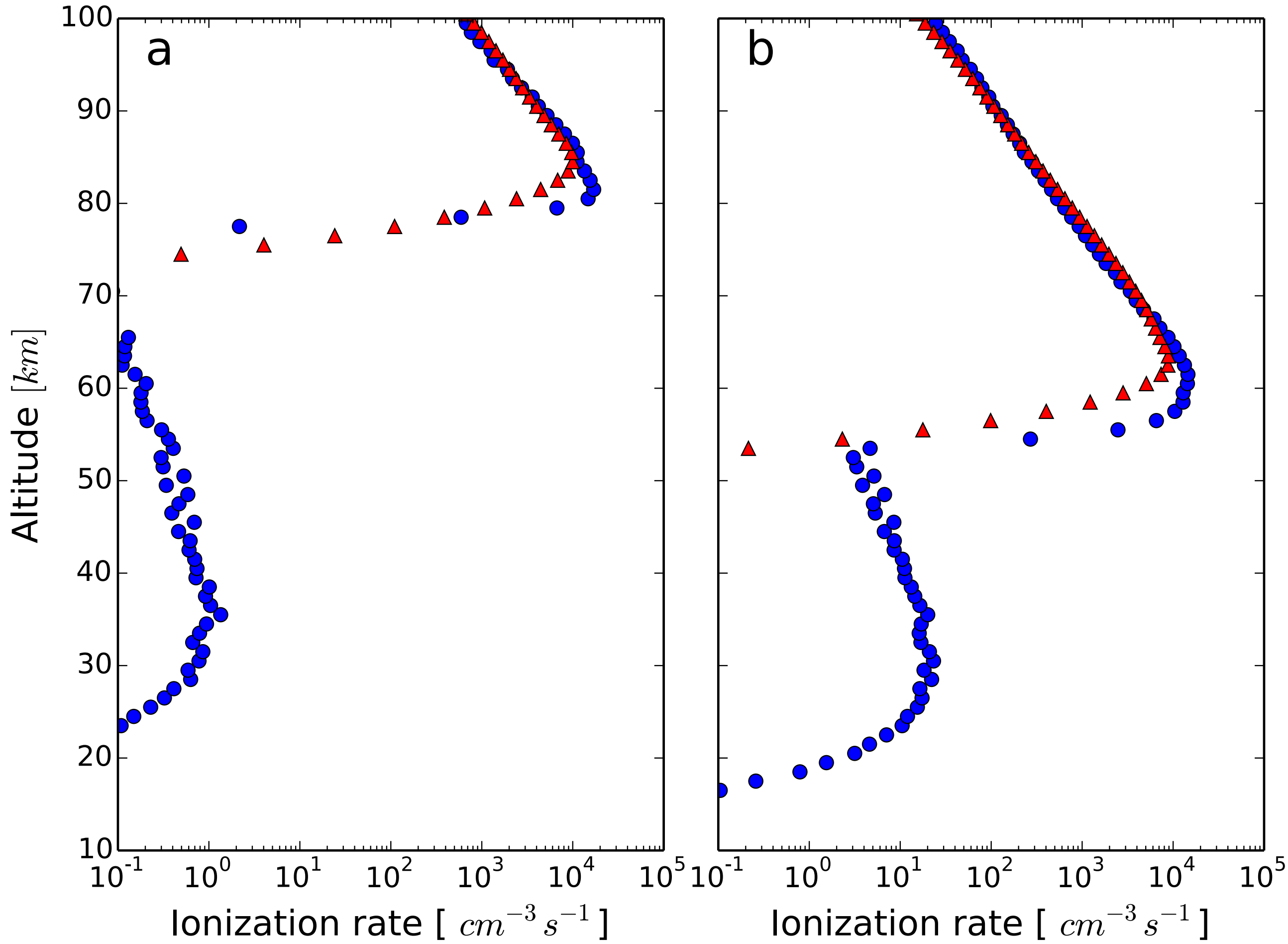

Fig. 2. Comparison of ionization yields for primary electrons with given energies as a function of the altitude above the sea level computed with the CRAC:EPII model (blue solid circles) and parametrization model (red solid triangles) according to Fang et al. (2010). a) electron flux of 1 erg $cm^{-2} s^{-1}$ with energy of 100 keV; b) electron flux of 1 erg $cm^{-2} s^{-1}$ with energy of 1 MeV. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

energy electron precipitation (e.g. Callis, 1991; Callis et al., 1996; Aikin and Smith, 1999; Turunen et al., 2009; Clilverd et al., 2010; Andersson et al., 2012; Krivolutsky and Repnev, 2012) an extension of parametrization models have been proposed (Millan and Thorne, 2007; Fang et al., 2010). Here we compare, for a several fixed energies of energetic electrons, our full physics Monte-Carlo model with a recent parametrization by (Fang et al., 2010) used, e.g., for computation of ionization due to particle precipitation (Huang et al., 2014).

We compare the ionization yields due to high energy precipitating electrons (monoenergetic electron fluxes of 1 erg $cm^{-2} s^{-1}$) entering into the atmosphere with that according to the model by Fang et al. (2010), for 100 keV and 1 MeV (Fig. 2). The CRAC:EPII model agrees almost perfectly with the parametrization model in the upper of the considered interval, viz. above 60–80 km, where ionization is driven by direct ionization losses. However, there is a slight difference in the ionization peak, which is predicted to be at a slightly lower altitude compared to the parametrization model, and its ionization rate is higher by 35–40%. The contribution of Bremsstrahlung photons to ionization is clearly seen at altitudes of about 30 km. The observed difference in the region of maximum ion production is due to a combination of various processes related to the complex high-energy electron propagation confined by the Monte Carlo model. In general, a good agreement between the two models is achieved, specifically in the upper atmosphere. We note that the agreement between our model and the one by Fang et al. (2010) is much better than the difference (up to an order of magnitude) between the two versions of the parametric model of Fang et al. (2008, 2010). Therefore, the CRAC:EPII is capable of assessing the ion production by high energy electron precipitation. The CRAC:EPII directly simulates, in contrast to parametrization models, contribution of Bremsstrahlung in the lower atmosphere, which is an important extension. In addition, minor discrepancy may arise from the neglected energy leakage for heating, and re-emission from excitation, in the optical range.

4. Spectrum of precipitating electrons and the derived ion production rate

Different methods have been proposed to estimate the spectrum of precipitating electrons (e.g. Clilverd et al., 2010; Neal et al., 2015; Whittaker et al., 2013; Wild et al., 2010). In general, it is possible to reconstruct the spectra from satellite-born measurements (e.g. Rodger et al., 2010, 2007; Peck et al., 2015). But this requires additional corrections as shown recently by Asikainen and Mursula (2013). A detailed description of the precipitating electron spectra is beyond the topic of this work.

Here we use the electron spectra obtained directly from balloon-born measurements (Bazilevskaya and Makhmutov, 1999), whose details are given elsewhere in this issue (Makhmutov et al., 2016). In general it is assumed that the flux of precipitating electrons at the top of the atmosphere is exponential:

$$J_e(K) = A_e \cdot \exp(-K/E_0) \tag{3}$$

(e.g. Millan et al., 2007; Comess et al., 2013). The characteristic

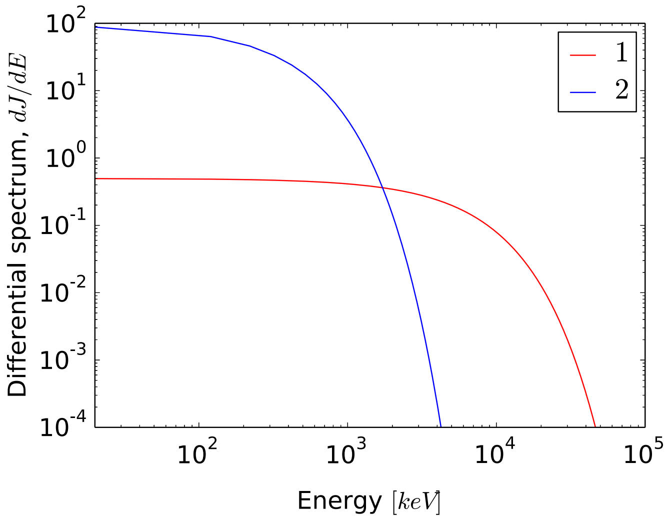

Fig. 3. An example of differential spectra of precipitating electrons. The spectra are derived independently on the basis of balloon measurement in the Murmansk region (Makhmutov et al., 2016).

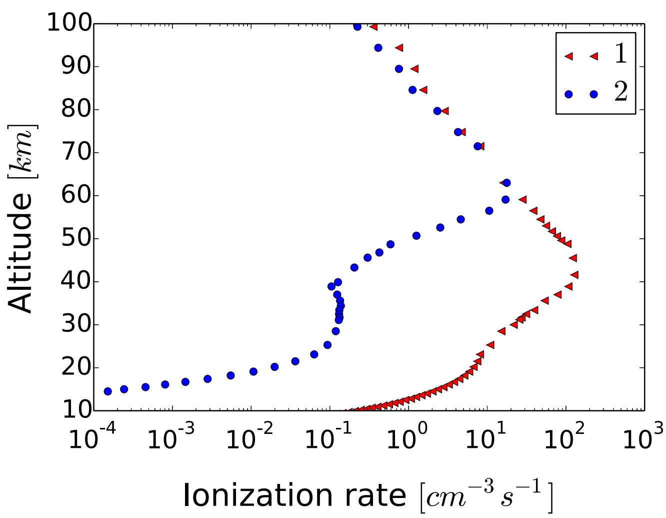

Fig. 4. Ion production rate for the example spectra Fig. 3 of precipitating electrons (07-Jan-2004, red triangles) and (30-Oct-2002, blue dots) computed with the CRAC:EPII model. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

energy E_0 is in the range a few keV up to a few MeV. The spectrum is reconstructed considering the characteristics of energetic electron precipitation in the polar atmosphere according to Makhmutov et al. (2003a). Here we give an example of the event spectrum derived independently by those authors on the basis of balloon measurement in Murmansk region (67°33′N, 33°20′E) on 30-October-2002 and 07-January-2004 (as shown in Fig. 3). The characteristics of the spectra in Eq. (3) are $A_e = 93.7\ \mathrm{cm^{-2}\,s^{-1}\,keV^{-1}}$, $E_0 = 3.09 \cdot 10^2$ keV and $A_e = 0.496\ \mathrm{cm^{-2}\,s^{-1}\,keV^{-1}}$, $E_0 = 5.45 \cdot 10^3$ keV, respectively. These spectra were used as an input in the CRAC:EPII model to estimate the ion production rate (Fig. 4). The derived ion production rate is in a good agreement with previous studies (Makhmutov et al., 2003a; Sloan et al., 2011). The contribution of Bremsstrahlung is clearly seen at altitudes below about 25 km for spectrum 1 and below 40 km for spectrum 2.

5. Conclusion

In this work we present a comparison of the Monte Carlo model for assessment of atmospheric ionization induced by precipitating energetic electrons with a parametrization model. The model is based on the formalism of response (ionization yield) functions, derived with extensive off-line Monte Carlo simulations. In contrast to a simplified parametrization models, it accounts explicitly for the contribution of Bremsstrahlung, which is important in the mid-lower atmosphere. Moreover, it greatly (up to 500 MeV) extends the energy range above 1 MeV, which is the maximum energy in many parametrization models (Fang et al., 2008, 2010). In addition, our model is flexible and user-friendly (specifically for operational purposes), because it is based on a widely used application-oriented formalism of ionization yields pre-computed in heavy simulation runs with high statistic.

We note that the present results show agreement (J. Wissing, personal communication, June 2015) with another Monte–Carlo model focused on satellite measurements, AIMOS (Wissing and Kallenrode, 2009; Wissing et al., 2011). A laborious direct comparison of these two models is planed for the future work, which should clarify technical uncertainties related to different atmospheric profiles, physical models involved and different code versions. A detailed study of various atmospheric profile parametrizations and/or particle generators within a same platform (tool) is discussed elsewhere (Mishev and Velinov, 2014).

The application of CRAC:EPII model for estimation of ionization yields for energetic electrons shows good agreement with a recent analytical parametrization model. The agreement is good in the upper part of the atmosphere (upper mesosphere – thermosphere), but the new model shows that the parameterization model may underestimate ionization in the middle atmosphere (lower mesosphere – stratosphere) because of the underaccounted Bremsstrahlung of energetic electrons.

As an example, the CRAC:EPII model was applied to compute the ion production rate in the upper atmosphere using a balloon-borne measured spectrum of precipitating electrons for two events of 30-October-2002 and 07-January-2004.

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