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Temporal 3D refined simulation of SF_6 release in the ionosphere

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Abstract

A number of significant studies have been dedicated to SF_6 releases. However, given the complicated nature, the simulations provided at the design phases are still not consistent with those diagnosed in experiments. It is mainly because the actual conditions of experiments have not been fully introduced in the state-of-art models. A temporal 3D refined simulation model of SF_6 release by a rocket payload is proposed in this paper. It first considers the release status (rocket attitude, velocity, etc.), release process (duration, injection velocity, the flux of the chemical release, etc.) and ambient neutral wind. This model is better than existing ones; the latter can only deal with release from a point source. The time-dependent drift of the released cloud, driven by the velocities of the rocket inertia and neutral wind, are calculated accurately. The non-uniform spherical structure of the electron density hole driven by the lasting release along the trajectory and the injection velocity are also described. The release flow field is calculated by using a new microcell method. The temporal 3D refined model proposed could be useful for improving the diagnosis and also helpful for the theory on chemical releases.

Keywords: Ionosphere; Chemical release; Simulation; Active experiment

1. Introduction

The evolution of ionospheric disturbances caused by chemical releases has been studied both experimentally and theoretically (e.g., Booker, 1961; Jackson et al., 1962; Perkins et al., 1973; Zabushky et al., 1973; Mendillo et al., 1975a, 1975b, 2008; Doles et al., 1976; Davis, 1979; Zinn et al., 1982; Klobuchar and Abdu, 1989; Sultan et al., 1992; Zhao et al., 2016). Among those, SF_6 is one of the best hole-making chemicals used to attach electrons and generate depletions. The chemistry and dynamics of SF_6 releases in the ionosphere were studied by Bernhardt (1979a, 1984) and Mendillo and Forbes (1978, 1982). Bernhardt (1982, 1988) investigated the plasma and fluid instabilities of ionospheric disturbance caused by SF_6 releases. Bernhardt et al. (1986) and Hunton et al. (1987) studied the excitation of airglow signatures by SF_6 releases. Scales and Bernhardt (1991) established the simulation model of the orbital SF_6 release. Hu et al. (2011) investigated the ionospheric disturbance and its effects on radio propagation produced by chemical release under various conditions.

A number of significant studies have been dedicated to SF_6 releases. However, given the complicated nature, the experimental results are inconsistent with the simulation, and sometimes, the disparity is very large. The one and two dimensional models for point source releases were proposed by Bernhardt (1984) and Hu et al. (2011). The release status (the rocket attitude and velocity, etc), release process (duration, injection velocity and the flux, etc) were ignored there, so the simulation of electron density holes were uniform spheres or ellipsoids. However, the symmetrical nozzles are usually adopted in order to maintain the force

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balance of rocket and payload during release. The gas is injected in two opposite directions. It will cause the released cloud to deviate from the spherical distribution, especially at early time. On the other hand, the rocket uninterruptedly releasing gas in nominal duration along its flight trajectory, so it generates a released cloud elongated in space. These factors will affect the release distribution and shape of the electron density hole. The errors will be inevitably brought if they are ignored. But, for both theoretical work and follow on campaign design, it is crucial to establish a temporal 3D refined simulation model.

A temporal 3D refined simulation model of SF_6 release by using a rocket payload is established in this paper. It firstly takes release status, release process and the ambient neutral wind into account. In addition, this new model uses a microcell method to calculate the released gas flow field. This model may be useful for improving the diagnosis and thus also helpful for studying ionospheric instabilities generated by chemical releases. The remainder of this paper is organized as follows. Section 2 discusses the chemistry and dynamics of SF_6 in the ionosphere, including its diffusion, chemical reaction, and plasma diffusion. The temporal 3D refined model, including a simulation process and a new microcell method of calculation of injected gas flow field, is established in Section 3. The numerical simulations are provided and discussed in Section 4. Finally, a brief summarization is provided in Section 5.

2. Chemistry and dynamics of SF_6 in the ionosphere

The chemistry and dynamics of SF_6 in the ionosphere is complex. It can be divided into several steps: expanding, freezing and evaporation of the injected gas, free diffusion. Initially, SF_6 cloud rapidly expands in a brief period (a few 10's of seconds) between the time of release and the time of diffusively controlled expansion, and consequently, SF_6 cloud temperature decreases sharply. When the density of SF_6 is extremely low, SF_6 stops condensation due to its nearly collisionless interaction with the ambient atmosphere. SF_6 is heated by the ambient atmosphere, and eventually, the injected gas reaches thermal equilibrium with the surrounding environment. Chemical reactions continue during all dynamics processes.

2.1. SF_6 diffusion

Assuming an unperturbed ambient atmosphere, the approximate solution to the gas diffusion equation of a point source release (Bernhardt, 1979b) is as follows:

$$n(x,y,z,t) = \frac{N_0}{(4\pi D_0 t)^{3/2}} \exp\left\{ -z\left(\frac{3}{4H_b}+\frac{1}{2H}\right) - \frac{H_b^2[1-\exp(-z/2H_b)]^2}{D_0 t} - lt - \frac{(x^2+y^2)e^{-\frac{z}{2H_b}}}{4D_0 t} - (\frac{1}{H_b}-\frac{1}{H})^2 \frac{D_0 t \exp(z/2H_b)}{4} \right\}, \tag{1}$$

where N_0 is the number of molecules released, D_0 is the injected gas diffusion coefficient at the point of release, n is the injected gas density, H is the injected gas scale height, H_b is the atmosphere scale height, and l is the injected gas reaction loss coefficient.

Table 1
Reactions stimulated by SF_6 release (selected from Bernhardt et al., 1986).

Reaction	Rate, cm^3/s
$SF_6 + e^- \underset{k_a}{\overset{k_1}{\leftrightarrow}} (SF_6^-) * \xrightarrow{k_b} SF_6^-$	$k_1 = 2.2 \times 10^{-7}/[1 + 640\exp(-4770/T)]$
	$k_a = 4.00 \times 10^4 s^{-1}$
	$k_b = k_a/10$
$SF_6 + e^- \xrightarrow{k_2} SF_5^- + F$	$k_2 = 2.2 \times 10^{-7} - k_1$
$SF_6^- + O^+ \xrightarrow{k_5} SF_6 + O^*$	$k_5 \approx 5 \times 10^{-8}$
$SF_5^- + O^+ \xrightarrow{k_6} SF_5 + O$	$k_6 \approx k_5$

2.2. Chemical reaction

The released gas will undergo several chemical reactions occurring simultaneously along with the dynamical processes. The major chemical reactions are listed in Table 1.

2.3. Plasma diffusion

Changes in electron density in the release area destroy the original structure of electron distribution and dynamic balance. Based on plasma diffusion theory, which assumes that plasma only moves along the magnetic field, the plasma diffusion equation (Hu et al., 2011) is given as follows:

$$\begin{aligned}\frac{\partial n_p}{\partial t} = {} & D_p \cdot \cos^2 I \cdot \frac{\partial^2 n_p}{\partial x^2} + D_p \cdot \frac{\cos I \cdot \sin I}{H_p} \cdot \frac{\partial n_p}{\partial x} \\ & - \cos I \cdot u_b \cdot \frac{\partial n_p}{\partial x} + D_p \cdot \sin^2 I \cdot \frac{\partial^2 n_p}{\partial z^2} \\ & + \left(\sin^2 I \cdot \frac{\partial D_p}{\partial z} + D_p \cdot \sin^2 I \cdot \frac{1}{T_p} \cdot \frac{\partial T_p}{\partial z} + D_p \cdot \sin^2 I \cdot \frac{1}{H_p} \right. \\ & \left. - \sin I \cdot V_b \right) \cdot \frac{\partial n_p}{\partial z} + \left(\sin^2 I \cdot \frac{\partial D_p}{\partial z} \cdot \frac{1}{T_p} \cdot \frac{\partial T_p}{\partial z} + \sin^2 I \cdot \frac{\partial D_p}{\partial z} \cdot \frac{1}{H_p} \right. \\ & \left. + D_p \cdot \sin^2 I \cdot \frac{\partial^2 \ln T_p}{\partial z^2} + D_p \cdot \sin^2 I \cdot \frac{\partial (1/H_p)}{\partial z} \right) \cdot n_p + P + L, \end{aligned} \tag{2}$$

where n_p is the plasma density; t is the time; P and L are the chemical production and loss terms, respectively; $T_p = (T_e + T_i)/2$ is the plasma temperature; $H_p = 2T_p k/(m_p g)$ is the plasma scale height; k is the Boltzmann constant; m_p is the plasma molecule mass; g is the gravitation acceleration; I is the magnetic field obliquity; D_p is the plasma ambipolar diffusion coefficient; and V_b is the neutral wind speed.

3. Modeling

The diffusion of the injected gas as well as the shape, size, and position of the electron density hole are affected