Stochastic Models of Hot Planetary Coronae

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Abstract. The uppermost layers of a planetary atmosphere are populated by the suprathermal particles produced in the transition region between the collision-dominated and free-molecular atmospheric layers under the forcing of solar ultraviolet radiation and of solar wind and magnetospheric plasma. This atmospheric region is called a hot planetary corona. We present a numerical stochastic model to investigate both the local formation and kinetics of suprathermal particles and their transport to exospheric heights from underlying atmospheric layers. In contrast to other commonly used approaches, the suggested numerical model is suitable for studying the flows of rarefied atmospheric gas weakly and strongly perturbed by suprathermal particles, i.e., for studying the formation of hot planetary coronae. Highly efficient Monte Carlo algorithms with statistical weights underlie the numerical implementation of the model basing on the DSMC method. The recent applications of this model are illustrated by investigation of the hot oxygen corona at Mars.

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INTRODUCTION

Hot Planetary Coronae

The uppermost layer of a planetary atmosphere, where the density of neutral particles is vanishingly low, is commonly called the exosphere or the planetary corona. Current theories of planetary coronae are based mainly on ground-based and space observations of exospheric emission features which together with *in situ* mass-spectrometer measurements allow the density and temperature height profiles of the exospheric components to be constructed. The measurements reveal that planetary coronae contain both a fraction of thermal neutral particles with a mean kinetic energy corresponding to the exospheric temperature and ***a fraction of hot neutral particles*** with mean kinetic energy much higher than the exospheric temperature [1,2].

These observations and models required a different description of the uppermost atmospheric layers than that provided by the thermal, collisionless models of planetary exospheres [1]. The existence of a hot atom component is a manifestation of the importance of non-thermal processes and such hot atoms are responsible for the atmospheric losses determining the evolution of planetary atmospheres under the astronomical timescales.

Suprathermal neutral atoms and molecules

Suprathermal (or hot) atoms and molecules are generally considered to be particles with kinetic energies above 5–10 kT, where T is the temperature of an ambient atmospheric gas. Such hot particles are produced in various physical and chemical processes whose products have an excess kinetic energy. Exothermic chemistry induced by the solar ultraviolet photons is accompanied by the release of energy on the order of several eVs [3]. Charge exchange and atmospheric sputtering induced by the solar wind, magnetospheric or pick-up ions can result in much larger energy transfers, producing hot particles with energies up to several hundred eVs [4]. If the production rate of the suprathermal particles is faster than thermalization, then a stable fraction of them is formed.

Suprathermal particles produced in upper atmospheric layers have been shown in the recent studies to play an important role in the chemistry and energetics of the upper atmosphere. Specifically, they: *(i) lead* to local changes in the chemical composition, because of the high non-equilibrium rate coefficients of the chemical reactions [5,6]; *(ii) produce* nonthermal atmospheric emission features [7]; *(iii) form* hot planetary coronae [5,8,9,10] and

enhance nonthermal atmospheric losses [2].

Numerical approaches

The following numerical approaches have been used to simulate nonthermal losses from planetary atmospheres (see, e.g., [2,11]): *(i) a multi-stream method* is commonly used only for systems with a weakly perturbed thermal state of the atmospheric gas; *(ii) finite-difference methods* that directly solve the Boltzmann kinetic equations for suprathermal particles. This approach is currently used only to analyze the local kinetics of the suprathermal particles; *(iii) a test-particle Monte Carlo method*, which is best suited also to the investigation of systems in which suprathermal particles perturb the thermal state of the gas only weakly; *(iv) a stochastic simulation method* [5,11], which modifies the Direct Simulation Monte Carlo (DSMC) method [12]. In contrast to the listed above methods, this stochastic approach is suitable for studying the flows of rarefied atmospheric gas both weakly and strongly perturbed by suprathermal particles, i.e., for studying the formation of hot planetary coronae.

STOCHASTIC MODELS

Kinetics of suprathermal (hot) particles

Let the rarefied gas of a planetary atmosphere be composed of α_i, $i=1,...,S$ atoms and molecules in a physical volume V. Each particle of the component α_i (an atom, a molecule, and/or their ion) has its own mass m_i, position $\boldsymbol{r_i}$ velocity $\boldsymbol{c_i}$, and set of quantum numbers $\boldsymbol{z_i}$ for each of the possible internal excitation level. These chemically distinct components collisionally interact through $m=1,...,M>1$ binary chemical reactions $\alpha_i + \alpha_j \rightarrow \alpha_k + \alpha_l$. For the generality of describing this chemically reactive system, we will consider reactions as a collisional process that includes both elastic ($\alpha_i = \alpha_k$ and $\alpha_j = \alpha_l$), and inelastic ($\alpha_i = \alpha_k$, $\alpha_j = \alpha_l$, but $\boldsymbol{z_i} \neq \boldsymbol{z_k}$ and/or $\boldsymbol{z_j} \neq \boldsymbol{z_l}$ internal excitation levels differ) and chemically reactive ($\alpha_i \neq \alpha_k$ and/or $\alpha_j \neq \alpha_l$) collisions. The probabilities of reactions are specified by the scattering functions $g_{ij} d\sigma_m$, where $d\sigma_m$ are the differential scattering cross section for reaction m, $g_{ij} = \left| \boldsymbol{c}_i - \boldsymbol{c}_j \right|$ is the relative velocity of colliding particles. The evolution of the suprathermal particles in a planetary atmosphere at the microscopic level of description can be determined by solving the system of Boltzmann kinetic equations

$$\frac{\partial F_{\alpha_i}}{\partial t} + \boldsymbol{c} \frac{\partial F_{\alpha_i}}{\partial \boldsymbol{r}} + \frac{\Gamma}{m_\alpha} \frac{\partial F_{\alpha_i}}{\partial \boldsymbol{c}} = Q_{\alpha_i} + \sum_m J_m^{\alpha_i} (F_{\alpha_i}, F_{\alpha_j}), \qquad (1)$$

together with initial and boundary conditions for the atmospheric gas in volume V subjected to the external force fields $\boldsymbol{\Gamma}$ of the planet [5,11]. Here, we describe the state of the gas by using the distribution functions for the gas particles by the velocity and internal excitation states $F_{\alpha_i}(t,\boldsymbol{r},\boldsymbol{c}) = n_{\alpha_i}(t,\boldsymbol{r},\boldsymbol{z}) f_{\alpha_i}(t,\boldsymbol{r},\boldsymbol{c})$, where $n_{\alpha_i}(t,\boldsymbol{r},\boldsymbol{z})$ is the particle number density in state $\boldsymbol{z}$, and $f_{\alpha_i}(t,\boldsymbol{r},\boldsymbol{c})$ is the single-particle velocity distribution function normalized to unity. The source functions $Q_{\alpha_i}(t,\boldsymbol{r},\boldsymbol{c})$ specify the suprathermal-particle production rates due to the exothermic chemistry and ion-induced atmospheric sputtering. The collision integrals $J_m^{\alpha_i}(F_{\alpha_i}, F_{\alpha_j})$ on the right-hand sides of the kinetic equations describe the change in gas state due to the elastic and inelastic collisions and are written in the standard form.

The chemical kinetics of a rarefied atmospheric gas at the microscopic level of description is completely determined by means of the dynamical and probabilistic characteristics of molecular collisions --- the scattering functions and the distributions of the colliding particles in translational and internal degrees of freedom. The chemical evolution of the atmospheric gas with the production of suprathermal particles has a complex structure of the kinetic rates of translational and internal energy exchange. The following characteristic cases occur:

a) Chemistry of suprathermal (hot) particles - a situation where suprathermal particles (hot subsystem) are a small admixture that weakly perturbs the thermal state of the ambient atmospheric gas (thermal subsystem), i.e., the source functions in (1) are much smaller than collision integrals. Thus, the thermal and hot subsystems are described by using the balance gasdynamic equations for the thermal components and the kinetic equations (1) for the suprathermal components, which contain the partially averaged collision integrals between particles of the different subsystems.

b) Microscopic non-equilibrium kinetics - a situation where the characteristic microscopic and macroscopic timescales of the change in parameters for all gas components are comparable. In this case, the state of the gas is determined by the solution of the basic system (1) of nonlinear kinetic equations, and, accordingly, the distribution functions depend explicitly on time.

The flow of gas in a planetary corona is most faithfully described either by a mixed kinetic system, where the perturbations of the thermal state of the ambient atmospheric gas by suprathermal particles are small, or by a completely kinetic system (1) of Boltzmann equations, where these perturbations are significant and the *planetary corona is hot*. A number of methods have been developed in the kinetic theory of rarefied gases to investigate the gas dynamics and kinetics in states close to the local thermal equilibrium [12]. Highly non-equilibrium systems are difficult to analyze because of the mathematical complexity of the Boltzmann kinetic equations (nonlinearity and high multiplicity of the collision integrals), which requires invoking new approaches.

A Numerical Kinetic Model for the Formation of a Hot Planetary Corona

A very promising approach is the development of discrete mathematical models that use the probabilistic interpretation of collisions in an ensemble of model particles. The Direct Simulation Monte Carlo (DSMC) method [12] and its modification for studying non-equilibrium processes in the planetary atmospheres [5,13] belong to this class of approaches. The basic idea of this approach to solving the system of Boltzmann equations (1) is to approximate the measures $F_\alpha(t,\mathbf{r},\mathbf{c})d\mathbf{r}d\mathbf{c}$ by a discrete numerical model with point measures -- a system or ensemble of model particles. A stochastic discrete model to investigate the formation, kinetics, and transport of suprathermal particles in a planetary corona should take into account the following peculiarities of the flow of atmospheric gas in the planetary corona:

- the local mean free time and path for suprathermal particles should be taken as the characteristic time and space scales at the molecular level of describing the state of the gas in the planetary corona;
- the parameters of the atmospheric gas change strongly in a hot planetary corona from the collision-dominated regime of gas flow in the dense thermosphere to the virtually collisionless (free-molecule) regime of flow in the exosphere;
- significant differences between the densities of the suprathermal particles produced in the chemical and magnetospheric plasma sputtering processes and the ambient atmospheric gas are commonly observed.

Therefore the following approaches must be used in constructing a numerical model of hot planetary coronae:

- the splitting of the solution of the basic kinetic system (1) in physical processes into the simulation steps for the suprathermal particle sources, the collisional thermalization of these particles, and the collisionless transport of suprathermal particles in the planetary corona on a discrete time scale;
- the stochastic simulation of the formation of suprathermal particles and their local kinetics by using analog Monte Carlo algorithms with statistical weights;
- the calculation of the collisionless paths of suprathermal particles in the planetary corona by using finite-difference algorithms.

The formation region of the hot corona, the transition region between the relatively dense thermosphere and the highly rarefied exosphere, is broken down into a finite set of coupled cells with the characteristic cell sizes assumed to be smaller than or equal to the local mean free path. These cells are populated with model particles in accordance with the initial and boundary conditions for atmospheric gas. Each model particle is characterized by the vector where the particle of type α has the geometrical coordinates $\mathbf{r}_i$, velocity $\mathbf{c}_i$, and statistical weight w_i; i.e., this vector is the discrete measure that corresponds to the distribution function $F_{\alpha_i}(t,\mathbf{r},\mathbf{c}) = n_{\alpha_i}(t,\mathbf{r},\mathbf{z})f_{\alpha_i}(t,\mathbf{r},\mathbf{c})$. According to the basic idea of the DSMC method the evolution of such discrete kinetic model in each discrete time step is splitted to the simulation steps of the *free particle transport* in entire region under study, and of the *local*

kinetics of the formation and collisional relaxation of suprathermal particles in each of the cells. During the step of the free-molecule transport the velocities of the model particles change under the effect of external force fields, while the statistical weights of the particles do not change at the stage of free transport. Under the step of the local kinetics of the formation and collisional relaxation of suprathermal particles the gas is assumed to be homogeneous within the cell, and, accordingly, the particle positions do not change in each of cells. This stage is broken down into two substeps when suprathermal particles are initially produced in each cell in accordance with the photochemical or plasma source functions and the collisions of model suprathermal particles with the ambient atmospheric gas are subsequently drawn in the discrete time interval by stochastic simulation [11-13]. It is worth to note, that a weight transfer technique was used to realize the collisions between the real number of atmospheric gas molecules and suprathermal particles because of the possible significant differences between the densities of the suprathermal particles and the ambient atmospheric gas.

The Stochastic Kinetic Equation for Suprathermal Particles

Basing on the theory of random processes, the evolution of the suprathermal particles in the atmospheric gas can be described by the following stochastic kinetic equation [5,11,13]

$$\frac{\partial}{\partial t}\varphi(\boldsymbol{X},t) = V^{-1}\sum_{m}\sum_{i,j}\int g_{ij}\,d\sigma_m\left[\varphi(\boldsymbol{X}_{ij}^{m},t) - \varphi(\boldsymbol{X},t)\right] \tag{2}$$

This equation is linear with respect to the probability density distribution $\varphi(\boldsymbol{X},t)$ for state $\boldsymbol{X}$ of the gas at time t and is called the stochastic (or master) kinetic equation for the chemical kinetics of a rarefied gas. The equation (2) describes the evolution of a homogeneous jump-like Markovian process [5,11,13].

The Analog Monte Carlo Method of Solving the Stochastic Kinetic Equation

The direct methods of solving the stochastic (master) kinetic equation consist in setting up and solving a system of equations for the probabilities of all possible paths of the state of a chemically reactive rarefied gas. Unfortunately, this direct procedure can be performed only for a few very simple chemical systems [14] and involves enormous computational difficulties for real systems of chemical reactions. The Monte Carlo method, which consists in generating a sample of paths for the state of a chemically reactive gas, is an efficient tool for studying complex chemical systems in the stochastic approximation. The path generation procedure is much simpler - a sequence of transitions between the states of a chemically reactive gas and transition-separating times should be drawn based on the proper probability distributions. Such procedure is an analog Monte Carlo algorithm for solving the stochastic kinetic equation (2). In the numerical realizations of the stochastic model the following recent developments in the theory and practice of DSMC method were used:

(i) an effective approximation of the majorant frequency [15], where the collision probability for the chosen pair is estimated from the maximum possible frequencies, is used in choosing the next transition;

(ii) the multichannel nature of the selected reaction is taken into account for the transition to be realized; i.e., this transition is treated as the simultaneous drawing of all possible (elastic, inelastic, and chemically reactive) channels for each of which the corresponding weight proportional to the ratio of the partial cross section for a given channel to the total cross section of the collisional process is transferred;

(iii) since the algorithmic steps of ejection in of the fresh suprathermal particles, in accordance with the source functions, and realization of the collisional transitions are accompanied by the formation of new model particles, it is necessary to control the total number of model particles in the numerical model. An efficient method for this control is the so-called clustering of model particles [16], where groups of model particles with similar parameters are combined into a single particle with weighted parameters. This procedure allows the total number of model particles to be controlled.

Since Eq. (2) and, accordingly, the analog Monte-Carlo method for its solution are linear, the dynamical, physical, and chemical parameters of the gas are calculated by averaging the realizations of the paths of the random process.

RESULTS AND CONCLUSIONS

The stochastic simulation method had been widely used to investigate the formation, kinetics, and transport of suprathermal particles in the hot planetary and satellite coronae [2,11,13]. This approach was first used to study the formation of the hot oxygen geocorona [5,6,9], with taking into account the exothermic chemistry and the precipitation of magnetospheric protons and high-energy O^+ ions from the ring current. A stochastic modeling approach was also applied to study the hot hydrogen corona at Jupiter [13] formed by electron precipitation and the induced exothermic chemistry. We extended these studies by considering the formation of the hot oxygen corona at Europa [10], a Jovian satellite, which is an example of a highly non-equilibrium near-surface atmosphere; and the hot nitrogen corona at Titan [17], a Saturnian satellite, when hot atoms and molecules of nitrogen are only a small admixture to the ambient thermal molecular nitrogen - the main atmospheric component of Titan.

A detailed description of applications of stochastic models to the investigation of the local collision kinetics and transport of hot atoms in a planetary corona is given in [10,11,13,17]. We merely note here that the modeling, which is implemented at the molecular level, leads to the accumulation of a detailed statistics regarding the velocity (kinetic energy) distribution of suprathermal particles. For example, Figure 1(a) convincingly shows that the main

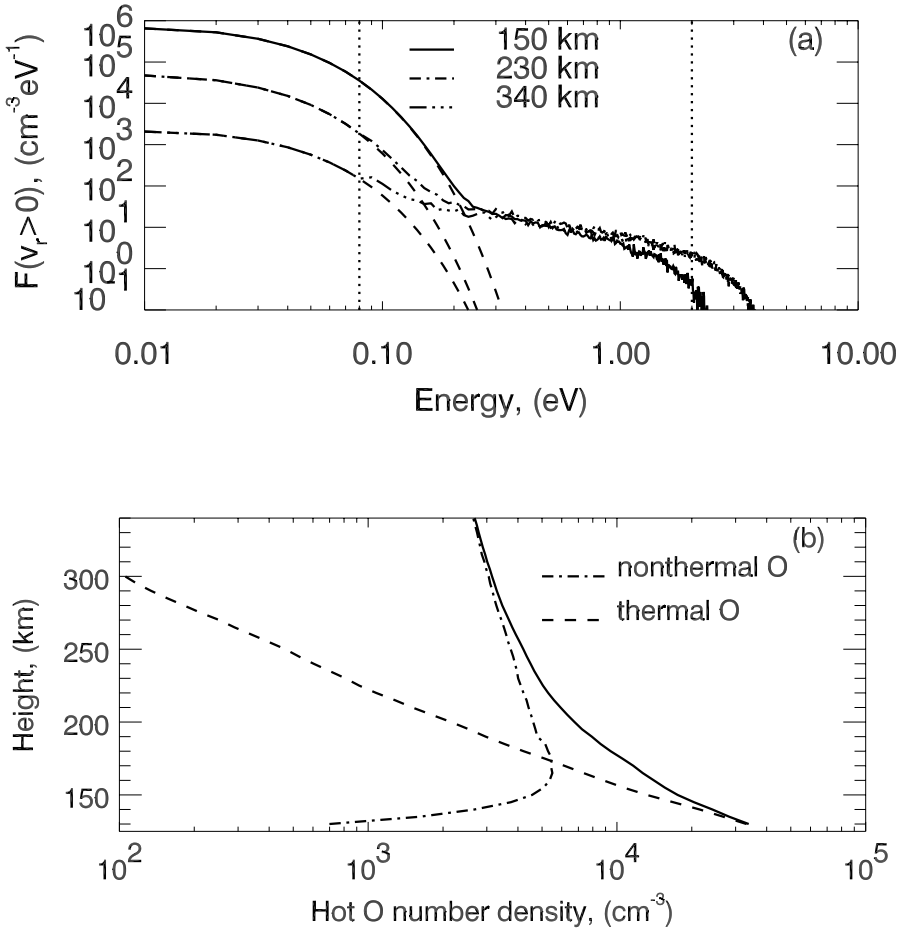

FIGURE 1. Hot oxygen corona at Mars: *(a)* Kinetic energy distribution functions $F(v_r > 0)$ of the upward moving thermal and nonthermal oxygen atoms at heights 150 (thermosphere), 230 (transition region near exobase), and 340 (exosphere) km are shown. Local equilibrium Maxwell distributions are given by dashed lines. The right vertical line shows the escape energy (~ 2 eV) for oxygen atoms in the Martian atmosphere. The left vertical line shows the energy ~ $5kT_n \approx 0.08$ eV above which oxygen atoms are suprathermal. *(b)* Height distributions of hot thermal (dashed line) and non-thermal (dash-dotted line) oxygen in the Mars upper atmosphere are shown. The total distribution is shown by solid line.

chemical source of hot oxygen atoms in the Martian atmosphere - the dissociative recombination of O_2^+ ions, - results in a substantial population of suprathermal O atoms, which is located between two vertical lines in Figure

1(a). The temperature of the Martian exosphere ranges from 200 K to 360 K depending on the solar activity level, therefore O atoms with kinetic energies above 0.08 - 0.1 eV were treated as suprathermal. This energy range is populated by oxygen atoms with energies just below the escape energy (~ 2 eV for Mars, right vertical line), which move on parabolic and elliptic trajectories and represent the hot oxygen corona at Mars. Upward moving oxygen atoms with kinetic energies above 2 eV form the non-thermal escape flux in the transition region of the Martian atmosphere. These escaping hot atoms are responsible for the oxygen loss rate from Mars [18].

The calculated density distribution in the corona is shown in Figure 1(b). It is seen that the main fraction of the hot corona at heights below the exobase (~ 200 km) is represented by atmospheric oxygen atoms from the suprathermal energy range in the local Maxwellian distribution. On the other side, above the exobase the main input is from non-thermal hot O atoms that are formed by dissociative recombination and reach exospheric heights. The total distribution of hot oxygen in the corona is shown by a solid line and indicates a much greater scale height than the ambient atmospheric gas.

We have presented a general scheme of the stochastic approach to investigating both the local formation and kinetics of suprathermal particles and their transport in the transition region between the collision-dominated and free-molecular regions of the upper planetary atmosphere. In contrast to other commonly used approaches, our approach allows us to investigate the flows of atmospheric gas both weakly and strongly perturbed by suprathermal particles in the transition regions of upper planetary atmospheres. These flows result in a formation of a hot planetary corona.

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