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Effects of exit boundary conditions on results of kinetic simulations of spherical expansion of mon- and diatomic gases in a gravitational field

Alexey N. Volkov

Department of Mechanical Engineering, University of Alabama, Tuscaloosa, AL 35487, USA

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ABSTRACT

The spherical expansion of mon- and diatomic gases in a spherically symmetric gravitational field is studied in kinetic simulations. The simulations are performed with the direct simulation Monte Carlo (DSMC) method in the range of the source Knudsen number, the ratio of the mean free path of gas molecules to the source radius, from 0.01 to 0.001, and in the range of the source Jeans parameter, the ratio of the characteristic gravitational binding energy of a gas molecule to its thermal energy, from 0 to 6. The exit boundary position R_1 of the computational domain was varied from 10 to 800 times the source radii R_0 in order to quantify the effect of the size of the computational domain and kinetic escape boundary conditions on the flow structure and escape rates. It is shown that the flow structure and escape rates for both mon- and diatomic gases are highly sensitive to the position of the exit boundary, when the source Knudsen number is sufficiently small and the source Jeans parameter corresponds to the transition from blow-off to Jean-like thermal escape. Outside the transitional range, the flow structures and escape rates are only marginally affected by the position of the exit boundary. In the case of a diatomic gas, the calculated flow structures converge with increasing size of the computational domain. In the case of a monatomic gas, the flow structures calculated for the transitional range of the Jeans parameter do not exhibit convergence with respect to increasing size of the computational domain in the considered range of R_1/R_0. It is shown that such flows remain subsonic and retain local equilibrium at arbitrary large distances from the source. The solution of the kinetic problem for a given molecular model in these conditions is uniquely defined by three parameters including the source Jeans parameter and Knudsen number and an additional parameter that constrains the flow far downstream. This additional parameter can be chosen in the form of the imposed number escape rate.

1. Introduction

The one-dimensional spherically symmetric gas outflow from a source with a gravitational field into vacuum is the simplest dynamical model describing the escaping atmosphere of a planetary body. This model is intensively used in astrophysics in order to predict atmospheric loss rates and structures of upper atmospheres of planetary bodies in the Solar system [1–5] and extrasolar planets [6–9]. The mechanism of the atmospheric loss in these conditions is usually called thermal escape, because the kinetic energy required for molecules to leave the atmosphere is ultimately provided by the thermal energy of the source. This is in contrast to non-thermal escape mechanisms, e.g., the heating of the atmosphere by stellar radiation, or sputtering atmospheric molecules by energetic particles from the solar wind [10]. For thermal escape, the flux of escaping molecules is composed of atmospheric particles whose kinetic energies are above the gravitational binding energy in the upper rarefied part of the atmosphere that is called the exosphere [11]. It is usually accepted that thermal escape occurs in either the blow-off or Jeans-like regime depending on the characteristic kinetic energy of gas molecules with respect to their gravitational energy [10,11], although the boundary between these regimes is not well-defined. In the blow-off regime, the initial enthalpy of fluid at the source surface is enough to leave the gravity well and the escaping atmosphere is characterized by large, usually supersonic, bulk gas velocity in the continuum part of the atmosphere. In the Jeans-like regime, the enthalpy of fluid is less than the depth of the gravity well and only a statistically small number of high-velocity molecules from the "tail" of the velocity distribution function leaves the atmosphere. In this case the outflow is supported by the upward heat flux maintained in the atmosphere.

During past six decades, the thermal escape problem was extensively studied with the continuum fluid models based on

E-mail address: avolkov1@ua.edu.

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simplified Navier–Stokes equations [1–3,6–9]. The deficiency of such models is in the application of continuum boundary conditions in the exosphere, where the gas flow is rarefied and the Navier–Stokes equations are no longer valid. In order to avoid this drawback, one can use kinetic models of the rarefied gas dynamics based on the Boltzmann or model, e.g. Bhatnagar–Gross–Krook, kinetic equations that can naturally account for the effects of rarefaction and non-equilibrium in the exosphere [11]. The majority of kinetic simulations of exospheric flows is performed with the direct simulation Monte Carlo (DSMC) method [4,5,12–17]. Applications of kinetic models to the thermal escape problem have shown that the transition from blow-off to Jeans-like escape occurs in a narrow transitional range of the Jeans parameter, the ratio of the gravitational binding energy to the thermal energy of a molecule at the source surface [14–16]. At small Knudsen numbers at the source surface, the ultimate manifestation of this sharp transition is the change in the number escape rate, number of molecules leaving the atmosphere per unit time, by orders of magnitude [14].

The kinetic models, however, also require kinetic escape boundary conditions at the exit boundary of the computational domain, which are usually based on the assumption that the flow above certain distance from the source occurs in the free molecular regime [13,15]. The applicability of these boundary conditions to flows in computational domains of finite sizes is not obvious, since the simulations show that at certain conditions thermally escaping flows are characterized by the relatively slow drop of the gas density and by the large size of the continuum flow zone.

The goal of this paper is to verify the applicability of the kinetic escape boundary conditions in systematic DSMC simulations of thermally escaping flows of mon- and diatomic gases with varying position of the exit boundary. The main finding obtained in these simulations is two-fold. First, the simulations showed that the flow structures and escape rates of both mon- and diatomic gases are sensitive to the position of the exit boundary in the range of the Jeans parameter that roughly corresponds to the transition from blow-off to the Jeans-like escape. Second, contrary to the flows of a diatomic gas, the flows of a monatomic gas in the transitional range of the Jeans parameter do not exhibit convergence with respect to increasing size of the computational domain in the considered range of the exit boundary position. This highly unexpected result is related to the fact that such flows remain subsonic and continuum at arbitrary large distances from the source, so that the kinetic escape boundary conditions do not allow one to obtain a unique flow structure and escape rate. In consequence, this observation means that the flow of a monatomic gas in the transitional range of the Jeans parameter is not uniquely defined by the parameters of the source and the molecular model, but also depends on an additional parameter that constrains the flow at infinitely far distance from the source.

2. Kinetic model of thermal escape

The kinetic model of spherically symmetric escaping atmosphere of a neutral gas is described in detail in a number of publications [15–17]. In this Section, therefore, only a brief description of the model is provided with the focus on the boundary conditions and non-dimensional similarity parameters used to describe the problem in reduced units.

In this paper, the kinetic simulations are performed for two molecular models. The flows of a monatomic gas (where the number ζ of internal degrees of freedom of a molecule is equal to zero) are simulated based on the Pseudo-Maxwellian (PM) model, where the intermolecular collisions are described by the Variable Hard Sphere model [18] with the viscosity index $\omega = 1$ and differential collision cross section $\sigma = \sigma_{\mathrm{ref}} c_{r,\mathrm{ref}}/c_r$ (c_r is the relative velocity for a pair of colliding molecules and $\sigma_{\mathrm{ref}} c_{r,\mathrm{ref}}$ is the model parameter). The flows of a diatomic gas with $\zeta = 2$ are simulated based on the combined Pseudo-Maxwellian–Larsen–Borgnakke (PMLB2) model, where the collision cross section is given by the PM model and the energy transfer between translational and rotational degrees of freedom is described by the Larsen-Borgnakke model [18,19]. In the case of the PMLB2 model, the probability of inelastic collisions (inverse collision number [18]) is assumed to be equal to 1. The case $\omega = 1$ is chosen for simulations because at temperatures ~100 K characteristic of upper atmospheres of distant planetary bodies in the Solar system, the viscosity index of major atmospheric species like N_2 is close to 1 [3,4].

Simulations of thermally escaping flows are performed with the DSMC method [18]. In the framework of this method, the computational domain, which represents a spherical layer between two concentric spherical surfaces placed at $r = R_0$ and $r = R_1$ (r is the radial distance from the source center), is divided into a one-dimensional mesh of cells, and the flow is described in terms of the motion of particles that simulate the gas molecules and are subject to the translational motion in the gravitational field of the source and binary collisions with each other. This method does not imply the explicit solution of a kinetic equation with respect to the distribution function of gas molecules, however, it has been shown that the DSMC method is a stochastic numerical method for estimating the functionals of solutions of the Boltzmann (or, for the gas of molecules with internal degrees of freedom, generalized Boltzmann [20]) kinetic equation [21].

Although the distribution function of the gas molecules is not necessary for implementation of the core of the DSMC algorithm, the boundary conditions for kinetic simulations still need to be formulated in terms of statistical distributions of parameters of individual gas molecules. Assuming a continuous distribution of energy of individual molecules with internal degrees of freedom and one-dimensional, spherically symmetric flow of a single component gas, the distribution function $f(r,v_{||},v_{\perp},\varepsilon_i,t)$ then depends on time t, radial distance from the source center r, parallel $v_{||}$ (along r) and perpendicular $v_{\perp}$ components of molecular velocity, and energy of internal degrees of freedom of an individual molecule ε_i. Any macroscopic gas parameter, including number density n, velocity u, parallel $T_{||}$, perpendicular $T_{\perp}$, and total T temperatures, temperature of the internal degrees of freedom T_i, the number, Φ_n, and energy, Φ_e, escape rates (number and total energy of molecules leaving the atmosphere per unit time) can be considered as a functional of $f(r,v_{||},v_{\perp},\varepsilon_i,t)$ [15,16].

In all simulations performed, it is assumed that at the source surface, $r = R_0$, molecules with $v_{||} > 0$ have a Maxwell–Boltzmann distribution with given number density n_0, zero velocity $u_0 = 0$, and temperature T_0, so that [18,22]

$$\text{For } v_{||} > 0: \quad f\left(R_0, v_{||}, v_{\perp}, \varepsilon_i, t\right) = \tilde{f}_{0t}\left(v_{||}, v_{\perp}\right)\tilde{f}_{0t}(\varepsilon_i) \tag{1}$$

$$\tilde{f}_{0t}\left(v_{||}, v_{\perp}\right) = \frac{n_0}{\left(2\pi k T_0/m\right)^{3/2}} \exp\left(-\frac{m\left(v_{||}^2 + v_{\perp}^2\right)}{2kT_0}\right)$$

$$\tilde{f}_{0t}(\varepsilon_i) = \frac{\varepsilon_i^{\zeta/2-1}}{\left(kT_0\right)^{\zeta/2}\Gamma(\zeta/2)} \exp\left(-\frac{\varepsilon_i}{kT_0}\right)$$

($\Gamma(x)$ is the gamma-function, k is the Boltzmann constant, and m is the mass of a molecule). Eq. (1) are referred to as evaporative-type boundary conditions, since they resemble the Hertz–Knudsen model describing surface evaporation [23], where molecules returning to this surface are assumed to be absorbed.