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Effective hydrodynamic hydrogen escape from an early Earth atmosphere inferred from high-accuracy numerical simulation

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ABSTRACT

Hydrodynamic escape of hydrogen driven by solar extreme ultraviolet (EUV) radiation heating is numerically simulated by using the constrained interpolation profile scheme, a high-accuracy scheme for solving the one-dimensional advection equation. For a wide range of hydrogen number densities at the lower boundary and solar EUV fluxes, more than half of EUV heating energy is converted to mechanical energy of the escaping hydrogen. Less energy is lost by downward thermal conduction even giving low temperature for the atmospheric base. This result differs from a previous numerical simulation study that yielded much lower escape rates by employing another scheme in which relatively strong numerical diffusion is implemented. Because the solar EUV heating effectively induces hydrogen escape, the hydrogen mixing ratio was likely to have remained lower than 1 vol% in the anoxic Earth atmosphere during the Archean era.

1. Introduction

The hydrodynamic escape of hydrogen driven by solar extreme ultraviolet (EUV) flux is a key process for controlling the evolution of the early Earth atmosphere and surface environment. For an atmosphere having a hydrogen-dominated upper layer, it was suggested that EUV heating energy is effectively transferred to mechanical energy of the outflow gas (e.g., Sekiya et al., 1980; Watson et al., 1981). Such effective escape, the rate of which can be limited by the diffusive separation rate of hydrogen across the homopause depending on the existing hydrogen mixing ratio (e.g., Walker, 1977), implies the rapid loss of hydrogen from early Earth and even possibly loss of entire water from Venus (e.g., Kasting and Pollack, 1983) under the enhanced EUV radiation emitted from the young Sun.

Early analytical studies of EUV-driven hydrodynamic escape investigated steady outflow solutions by solving simultaneous ordinary differential equations in the radial coordinate considering time derivatives to be zero in the conservation equations of mass, momentum, and energy with spherical symmetry. This approach sometimes faces difficulty in finding transonic solutions to avoid mathematical singularity. Numerical time integration of conservation equations is a possible approach to resolve this problem.

By performing this calculation, Tian et al. (2005a) reported escape rates significantly lower than those estimated by earlier studies. Their calculation was performed at a temperature as low as 250 K at the base of hydrogen-dominated region, which is presumably possible by effective cooling from a radiatively active secondary species. The obtained low escape rates would be attributed to the conductive loss of EUV heating energy toward the cold atmospheric base. Equating an estimate of the volcanic hydrogen degassing rate with the calculated escape rates, it was proposed that the early Earth atmosphere would be hydrogen rich with an H_2 mixing ratio as high as nearly 30%, even at 2.5 Ga. This significantly differs from the earlier estimates predicting an H_2 mixing ratio less than ~0.1 vol% during the Archean era (e.g., Walker, 1978).

Tian et al.'s numerical model, however, requires further testing for accuracy. In another paper (Tian et al., 2005b) they mentioned that their model scheme may have a difficulty in satisfying the radial uniformity of mass flux integral (taken over a sphere concentric with Earth) in steadily expanding isothermal solutions. This violation of the law of conservation of mass especially emerges at low altitudes in simulations with low atmospheric temperatures.

To avoid numerical instability, Tian et al. (2005a, 2005b) used the Lax–Friedrichs (LF) scheme, which introduces an artificial numerical diffusion (LeVeque, 1992; de Sterck et al., 2001). At low altitudes, the atmospheric density profile approximately

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follows hydrostatic equilibrium. At low atmospheric temperature, the density contrast between altitudes in the lower atmosphere becomes significant owing to the decrease in atmospheric scale height. If the LF scheme is applied to such a system, the artificial numerical diffusive flux, approximately equivalent to that by a diffusion process with diffusivity given by the sound speed times the grid interval, may sometimes overwhelm the true mass flux, particularly at low atmospheric altitudes. This calculation would thus cause a violation of the law of conservation of mass. On the other hand, calculated mass fluxes at the upper boundary are in good agreement with the analytical solution by Parker (1963), which is the main reason for using the LF scheme by Tian et al. (2005a, 2005b).

It is still unclear whether the LF scheme adequately reproduces the escape rate even for non-isothermal atmosphere. At least, the problem with mass conservation in the lower altitudes implies significant errors in estimating energy balance in the outflow gas. Therefore, this study will simulate the EUV-driven hydrodynamic escape of hydrogen by using a more reliable numerical scheme.

We have developed a new numerical model that adopts the constrained interpolation profile (CIP) scheme (Yabe and Aoki, 1991; Yabe et al., 2001b), a high-accuracy method for solving advection equations. The advantage of the CIP scheme is that it causes few numerical dispersion errors by predicting the advection of both numerical values and their gradients at each grid point. Because of this nature and numerical stability, the CIP scheme is considered to be an adequate method to simulate atmospheric outflow.

2. Model

Following Tian et al. (2005a), the hydrodynamic flow of an ideal gas atmosphere composed of pure H_2 with radial symmetry is described by the inviscid Eulerian equations

$$\frac{\partial(\rho r^2)}{\partial t}+\frac{\partial(\rho u r^2)}{\partial r}=0, \tag{1}$$

$$\frac{\partial(\rho u r^2)}{\partial t}+\frac{\partial(\rho u^2 r^2+pr^2)}{\partial r}=-\rho GM+2pr, \tag{2}$$

$$\frac{\partial}{\partial t}\left[\left(\frac{\rho u^2}{2}+\frac{p}{\gamma-1}\right)r^2\right]+\frac{\partial}{\partial r}\left[\left(\frac{\rho u^2}{2}+\frac{\gamma p}{\gamma-1}\right)ur^2\right]=-\rho uGM+qr^2+\frac{\partial}{\partial r}\left(\kappa r^2\frac{\partial T}{\partial r}\right), \tag{3}$$

where r is the distance from the center, u is the radial velocity; ρ, p, T are the gas density, pressure, and temperature, respectively. γ is the ratio of specific heats considered as 7/5, G is the gravitational constant, M is the mass of the Earth, κ is the thermal conductivity, and q is the heating rate. The equation of state is given by that of the ideal gas composed of pure H_2. The thermal conductivity is given by

$$\kappa=\kappa_0\left(\frac{T}{T_0}\right)^s, \tag{4}$$

where T_0 is the reference temperature, κ_0 is the thermal conductivity at $T=T_0$ and s is the constant power index. We set $T_0=250$ K, $\kappa_0=1.62\times10^{-1}$ J/m s K, and $s=0.7$ (Hanley et al., 1970).

The heating rate q is calculated by the same method used by Tian et al. (2005a, 2005b), which numerically solves the 2D radiative transfer of solar EUV flux incident from the solar direction into the spherically expanded atmosphere, and then laterally averages the energy absorption to obtain the radial heating profile at each time step. The EUV spectrum and the absorption cross section are provided by Woods and Rottman (2002) and Avakyan et al. (1998), respectively, for wavelengths shorter than 105 nm. To express the early solar EUV flux, the present-day time-averaged EUV spectrum is multiplied by enhancement factors neglecting the possible change in the spectrum profile. Furthermore, the heating efficiency of absorbed energy is considered as 0.15 (Watson et al., 1981). The temperature at the lower boundary is fixed at 250 K. Each of these settings is basically the same as those used by Tian et al. (2005a).

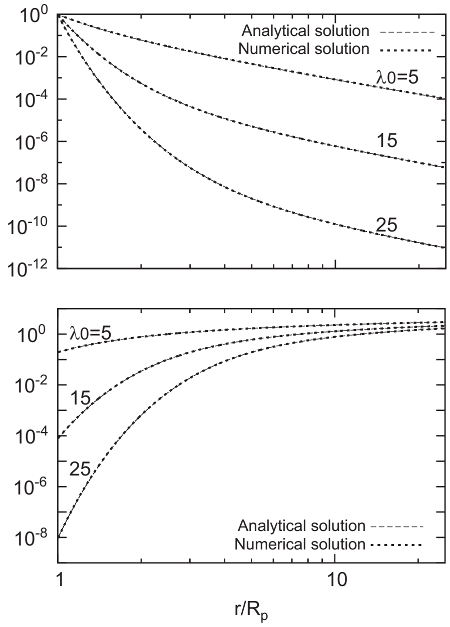

Fig. 1. Comparison of analytical solutions and numerical ones for the isothermal steady expansion of the atmosphere. Radial density (top panel) and velocity profiles (lower panel) are scaled by the basal density and sound velocity, respectively. Independent of the escape parameter over this range (taken at 5, 15, and 25), the numerical solutions are indistinguishable from the analytical ones.

Eqs. (1)–(3) are solved by explicit integration about time until the physical quantities settle into steady profiles. To perform time integration, we employ CIP schemes that are known to perform stable numerical integration of advection terms with a high degree of accuracy using reasonable computational resources. We adopted the CIP-CSL2 scheme (Yabe et al., 2001a) to solve the mass conservation equation because this method is optimized to guarantee the conservation of mass. To save computational resources, the original CIP scheme (Yabe and Aoki, 1991) is adopted for the advection terms of the momentum equation and the energy equation. The diffusion term in the energy equation is expressed by the centered difference formula. The upper and lower boundaries are set at $r=25$ Earth radius (6.36×10^3 km) and $r=6.46\times10^3$ km (the Earth radius + 100 km), respectively. The interval was divided into 1000 numerical grids with the grid-to-grid intervals exponentially increasing with r.

In each simulation run, the atmospheric density and temperature at the lower boundary are fixed as a parameter as well as the EUV enhancement factor. The other physical quantities in the lower and upper boundaries are estimated by linear extrapolations from the calculated domain. The initial density profile is given by the isothermal hydrostatic structure for the lower layer and is proportional to r^{-2} in the upper layer beyond an arbitrary radius. A constant velocity of 10^{-5} m/s is set as the initial velocity profile.

3. Results

3.1. Testing isothermal calculation

To test the performance of our model, we simulated the steady expansion of the isothermal atmosphere into the vacuum and