Escape of exoplanet atmospheres

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1 Planetary effective temperature

The effective (surface) temperature T_p of an exoplanet can be derived from

$$\pi R_p^2(1-A_B)\left(\frac{R_*}{a}\right)^2\sigma_{SB}T_*^4 = 4\pi R_p^2\frac{1}{f_R}\sigma_{SB}T_p^4 - L_{int} \tag{1}$$

where R_p is the radius of the planet, A_B is the Bond albedo, R_* is the radius of the host star, a is the orbital distance, σ_{SB} is the Stefan-Boltzmann constant, T_* is the effective temperature of the host star, f_R is the redistribution parameter of the atmosphere ($f = 1$ for isotropic emission, $f = 2$ for dayside emission only and $f = 4$ for instantaneous emission) and L_{int} is the internal luminosity of the planet. This relationship simply represents a balance between the absorbed stellar radiation and planetary emission. Assuming that $L_{int} = 0$, the effective temperature of the planet is simply

$$T_p = T_*\left(\frac{R_*}{2a}\right)^{1/2}\left[f_R(1-A)\right]^{1/4}. \tag{2}$$

2 Atmospheric structure

A simple relationship for pressure p and radius r in the atmosphere is derived from the equation of hydrostatic equilibrium:

$$\frac{1}{p}\frac{\partial p}{\partial r} = -\frac{GM_pm(r)}{kT(r)r^2} \tag{3}$$

where M_p is the planet mass, $m(r)$ is the mean molecular weight and we assumed a spherically symmetric gravity field. The quantity

$$H(r) = \frac{kT(r)}{m(r)g(r)} = \frac{kT(r)r^2}{GM_pm(r)} \tag{4}$$

is known as the pressure scale height. Assuming that T and m are constant, this equation can be integrated to give

$$p(r) = p(r_0)\exp\left[X(r) - X(r_0)\right] \tag{5}$$

where the parameter X known as the thermal escape parameter (see below) is

$$X = \frac{GM_p m}{kTr} = \left(\frac{V_{esc}}{V_T}\right)^2 = \frac{r}{H(r)} \tag{6}$$

and the escape velocity and most probable (thermal) speed are

$$\begin{aligned} V_{esc} &= \sqrt{\frac{2GM_p}{r}} \\ V_T &= \sqrt{\frac{2kT}{m}}. \end{aligned}$$

3 Exobase

The exobase is the outer edge of the atmosphere, by definition the altitude where the atmosphere becomes practically collisionless. Typically, it is taken to be the level where the mean free path between collisions S_m is roughly equal to the pressure scale height of the atmosphere i.e., for a single species:

$$S_m = \frac{1}{\sigma_c n_c} \approx H_c \rightarrow \sigma_c n_c H_c \approx 1 \tag{7}$$

where σ_c is the collision cross section, n_c is the 'critical' exobase density and H_c is the scale height at the exobase. This condition can also be written approximately in terms of the collision frequency $\nu_c \approx \sigma_c n_c V_{Tc}$ as

$$\frac{\nu_c H_c}{V_{Tc}} \approx 1. \tag{8}$$

Assuming an isothermal atmosphere with constant composition, we can write equation (5) as

$$\ln\left[\frac{X(r_c)}{\sigma_c r_c n(r_0)}\right] = X(r_c) - X(r_0), \tag{9}$$

which can be solved for the exobase radius r_c and thus $X(r_c)$ if T and m are known. If T and m change with altitude, equation (5) is not valid and equation (3) has to be integrated numerically.

4 Jeans escape

Jeans escape is a kinetic escape mechanism that applies at the exobase. The fluid flow velocity of species s is given by the velocity distribution function F_s as:

$$m_s n_s \mathbf{u}_s = m_s \int_\infty \mathrm{d}^3 v_s \mathbf{v}_s F_s(t, \mathbf{r}, \mathbf{v}_s) \tag{10}$$

where the velocity space volume element is

$$\mathrm{d}^3 v_s = -v_s^2 \mathrm{d}(\cos\theta)\mathrm{d}v_s \mathrm{d}\phi. \tag{11}$$

We write the flux of particles escaping through the upper hemisphere (with $\cos\theta$ ranging from 1 to 0) in spherical symmetry based on the outward radial component of the velocity vector:

$$\begin{aligned} n_s w_s &= -2\pi \int_{v_{esc}}^\infty v_s^2 \mathrm{d}v_s \int_1^0 v_s \cos\theta \mathrm{d}(\cos\theta) F_s \\ &= 2\pi \int_{V_{esc}}^\infty v_s^3 \mathrm{d}v_s \int_0^1 \cos\theta \mathrm{d}(\cos\theta) F_s \\ &= \pi \int_{V_{esc}}^\infty v_s^3 \mathrm{d}v_s F_s. \end{aligned} \tag{12}$$

4.1 Basic Jeans escape

In order to derive the formula for basic Jeans escape of neutral particles, we assume that the velocity distribution function is Maxwellian:

$$F_s(t, r, v_s) = n_s \left(\frac{m_s}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m_s v_s^2}{2kT}\right), \tag{13}$$

which gives the Jeans flux:

$$n_s w_{sJ} = \pi n_s \left(\frac{m_s}{2\pi kT}\right)^{3/2} \int_{V_{esc}}^\infty v_s^3 \exp\left(-\frac{m_s v_s^2}{2kT}\right) \mathrm{d}v_s. \tag{14}$$

The integral can be done by parts:

$$\begin{aligned} &\int_{V_{esc}}^\infty v_s^3 \exp\left(-\beta_s v_s^2\right) \mathrm{d}v_s = \int_{V_{esc}}^\infty v_s^2 v_s \exp\left(-\beta_s v_s^2\right) \mathrm{d}v_s \\ = &-\left[\frac{v_s^2}{2\beta_s} \exp\left(-\beta v_s^2\right)\right]_{V_{esc}}^\infty + \int_{V_{esc}}^\infty \frac{v_s}{\beta_s} \exp\left(-\beta_s v_s^2\right) \mathrm{d}v_s \\ = &\frac{1}{2\beta_s} V_{esc}^2 \exp\left(-\beta_s V_{esc}^2\right) + \frac{1}{2\beta_s^2} \exp\left(-\beta_s V_{esc}^2\right) \\ = &\frac{1}{2\beta_s^2}(X_s + 1)\exp(-X_s) = \frac{1}{2}\left(\frac{2kT}{m_s}\right)^2 (X_s + 1)\exp(-X_s) \end{aligned} \tag{15}$$

where

$$X_s = \beta_s V_{esc}^2 \tag{16}$$

Thus we can write Jeans flux at the exobase as:

$$\begin{aligned} n_{sc} w_{scJ} &= n_{sc} \pi \left(\frac{m_s}{2\pi k T_c} \right)^{3/2} \frac{1}{2} \left(\frac{2kT_c}{m_s} \right)^2 (X_{sc}+1) \exp(-X_{sc}) \\ &= n_{sc} \frac{1}{2\sqrt{\pi}} \sqrt{\frac{2kT_c}{m_s}} (X_{sc}+1) \exp(-X_{sc}) . \end{aligned} \tag{17}$$

Thus the global Jeans mass loss rate is

$$\dot{M}_J = 4\pi r_c^2 \sum_s \rho_{sc} w_{scJ} = 4\pi r_c^2 \sum_s \frac{\rho_{sc} V_{Tsc}}{2\sqrt{\pi}} (X_{sc}+1) \exp(-X_{sc}) \tag{18}$$

where $\rho_{sc} = m_s n_{sc}$.

4.2 Modified Jeans escape

Jeans escape assumes zero bulk flow through the exobase. If the bulk velocity of the atmosphere is u, the velocity distribution function at the exobase is the drifting Maxwellian:

$$F_s(t, r, v_s) = n_s \left(\frac{m_s}{2\pi k T} \right)^{3/2} \exp\left[-\frac{m_s}{2kT} (v_s - u)^2 \right] . \tag{19}$$

Integrating this over the appropriate velocity space as before gives the ratio of the modified Jeans escape rate to the basic Jeans escape rate (e.g., Volkov et al., 2011):

$$\frac{\dot{M}_{Js,mod}}{\dot{M}_{Js}} = \frac{0.5 \exp[-(Y_s+X_s)] + \left(\sqrt{Y_s X_s} + Y_s - 0.5\right) \exp\left[-(\sqrt{X_s} - \sqrt{Y_s})^2\right] + \sqrt{\pi} Y_s^3 \left[1 - \mathrm{erf}(\sqrt{X_s} - \sqrt{Y_s})\right]}{Y_s (1+X_s) \exp(-X_s)} \tag{20}$$

where the 'bulk escape parameter' is

$$Y_s = \left(\frac{u}{V_{Ts}} \right)^2 \tag{21}$$

and we dropped the use of the subscript 'c' for the critical level that is assumed throughout. Yelle (2004) used the modified Jeans escape rate as the upper boundary condition in his exoplanet escape model.

5 Equations of motion for hydrodynamic escape

The basic radial equations of motion for continuity of mass, momentum and energy, respectively, for the neutral atmosphere are:

$$\frac{\partial\rho}{\partial t}+\frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho w r^2\right) = 0 \tag{22}$$

$$\frac{\partial(\rho w)}{\partial t}+\frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho w^2 r^2\right) = -\frac{\partial\phi_g}{\partial r}-\frac{\partial p}{\partial r}+F_\mu \tag{23}$$

$$\frac{\partial(\rho c_v T)}{\partial t}+\frac{\partial}{\partial r}\left(\rho w r^2 c_v T\right) = \rho\left(Q_{\mathrm{Heat}}+Q_{\mathrm{Cool}}\right)-p\frac{1}{r^2}\frac{\partial}{\partial r}\left(w r^2\right)+\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\kappa\frac{\partial T}{\partial r}\right)+\Phi_\mu \tag{24}$$

where ρ is mass density, w is vertical velocity, ϕ_g is the gravitational potential, F_μ is a force due to viscosity, c_v is the specific heat capacity at constant volume, w is vertical velocity, Q_{Heat} is the specific (radiative) heating rate (per unit mass), Q_{Cool} is the specific (radiative) cooling rate, κ is the coefficient of heat conduction (see below) and Φ_μ is the volume heating rate by viscous dissipation. It is handy to consider different escape mechanisms and rates from the point of view of the energy balance in the upper atmosphere. The second term in the l.h.s of the energy equation describes radial advection of energy and the terms on the r.h.s describe net (radiative) heating, adiabatic expansion or contraction, conduction of heat and viscous dissipation, respectively.

Ignoring F_μ, the can write the momentum equation as

$$w r^2\frac{\partial p}{\partial r} = -\left[w r^2\frac{\partial}{\partial t}(\rho w)+w\frac{\partial}{\partial r}\left(\rho w^2 r^2\right)+w r^2\frac{\partial\phi_g}{\partial r}\right], \tag{25}$$

substitute it into equation (24) and use the equation of continuity to obtain

$$\frac{\partial}{\partial t}\left[F_\rho\left(c_v T+\frac{1}{2}w^2\right)\right]+\frac{\partial}{\partial r}\left[F_\rho\left(c_p T+\frac{1}{2}w^2+\phi_g\right)\right] = \rho r^2\left(Q_{\mathrm{Heat}}+Q_{\mathrm{Cool}}\right)$$
$$+\frac{\partial}{\partial r}\left(r^2\kappa\frac{\partial T}{\partial r}\right)+r^2\Phi_\mu \tag{26}$$

where $c_p = c_v + R$ and $F_\rho = \rho w r^2$ is the mass flux constant.

6 Stellar XUV heating and conduction

Assume that the energy balance in the upper atmosphere is between stellar XUV heating and conduction. In that case the flux of energy through the upper atmosphere is

$$F = -\kappa\frac{\mathrm{d}T}{\mathrm{d}r} = -A_k T^s\frac{\mathrm{d}T}{\mathrm{d}r} \tag{27}$$

where κ is the coefficient of heat conduction and the parameters for A_k and s are tabulated for different gases. For example, $A_k = 252\times10^{-5}$ W m^{-1} K$^{-(s+1)}$ and $s = 0.751$

for molecular hydrogen. Let us assume, naively, that the incoming stellar XUV flux supports a constant temperature gradient in the region $(r-r_0)$. Thus

$$A_k \int_{T_0}^{T} T'^{s} \mathrm{d}T' = F \int_{r_0}^{r} \mathrm{d}r' = F \int_{p}^{p_0} H \frac{\mathrm{d}p'}{p}. \tag{28}$$

Now, if we write $H \approx T H_0 / T_0$, we get

$$A_k \frac{T_0}{H_0} \int_{T_0}^{T} T'^{s-1} \mathrm{d}T' = F \int_{p}^{p_0} \frac{\mathrm{d}p'}{p'}, \tag{29}$$

which is easily solved to give

$$T(p) = \left[T_0^s + \frac{\epsilon F_{XUV} H_0 s}{4 A_k T_0} \ln\left(\frac{p_0}{p}\right)\right]^{1/s} \tag{30}$$

where we assumed that the incoming stellar flux is globally averaged, ϵ is the heating efficiency and $\ln(p_0/p) \approx 6.9$ seems to work for giant planets like Saturn (Koskinen et al., 2015).

7 Energy-limited escape

Once the escape parameter becomes small, the balance of net heating and conduction breaks down and the atmosphere begins to undergo rapid (hydrodynamic) escape. Under these circumstances, the adiabatic and the advection terms in the energy equation (24) become important. The advection term is really only significant at supersonic velocities, so in practice this means that the energy balance holds between the net heating and the adiabatic term. Integrating equation (26) in steady state from r_0 to infinity, we have

$$-F_\rho \left(c_p T - \frac{1}{2} u^2 + \phi_g \right) = \int_{r_0}^{\infty} r^2 \alpha(r) q(r) \mathrm{d}r = \epsilon F_E r_E^2 \tag{31}$$

where u is the bulk flow velocity at infinity, $\alpha(r)$ is the altitude-dependent heating efficiency, $q(r)$ is the volume energy deposition rate, ϵ is the column-averaged heating efficiency, F_E is the flux of energy per solid angle, and r_E is the effective radius of energy deposition. Assuming spherically symmetric point mass gravity, we have

$$-F_\rho \left(c_p T_0 - \frac{1}{2} u^2 - \frac{G M_p}{r_0} \right) = \epsilon F_E r_E^2. \tag{32}$$

For monatomic gas ($m c_p = 5/2 k T$), the thermal escape parameter would have to be lower than 5/2 at the base of the solution for the thermal energy term to be significant. The kinetic energy term, on the other hand, is only comparable to the thermal energy term for strongly supersonic final velocities. Thus we can write

$$F_\rho = \frac{\epsilon F_E r_E^2 r_0}{GM_p} \to \dot{M}_E = \frac{4\pi r_E^2 r_0 \epsilon F_E}{GM_p}. \tag{33}$$

Assuming that $r_E = r_0 = R_p$ and that the flux of energy is the incoming stellar XUV flux distributed globally around the planet, we obtain

$$\dot{M}_E = \frac{\pi \epsilon F_{XUV} R_p^3}{GM_p} \left(\frac{R_s}{a}\right)^2 \tag{34}$$

where F_{XUV} is the XUV flux at the stellar surface, R_s is the radius of the star and a is the orbital distance. This is the basic expression of energy-limited escape, which, in addition to the stellar luminosity, is proportional to $R_p^3/(M_p a^2)$ that we can easily evaluate for transiting planets.

8 Roche lobe overflow

In the above derivation of energy-limited escape, we assumed that the gravitational potential is spherical and due to the planet only. This is not accurate if the planet is very close to the star and 'Roche lobe overflow', driven by stellar gravity, is important. Let us define a coordinate system centered at the planet, with the y axis pointing in the direction opposite to the orbital motion of the planet, the x axis pointing from the planet to the star and the z axis pointing in the direction of the orbital angular momentum vector. The Roche potential in this system is

$$\phi_R(x,y,z) = -\frac{GM_p}{\left(x^2+y^2+z^2\right)^{1/2}} - \frac{GM_s}{\left[(a-x)^2+y^2+z^2\right]^{1/2}} - \frac{1}{2}\Omega^2 \left[(x-\mu a)^2+y^2\right] \tag{35}$$

where a is the orbital distance, M_s is the mass of the star, Ω is the orbital angular rotation rate (we assume tidal locking for the planet) and μ is the reduced mass of the system. In spherical polar coordinates centered at the planet, we have

$$\begin{aligned} x &= r\cos\phi\sin\theta = r\lambda \\ y &= r\sin\phi\sin\theta = r\xi \\ z &= r\cos\theta = r\nu \end{aligned}$$

and

$$\phi_R(r,\theta,\phi) = -\frac{GM_p}{r} - \frac{GM_s}{\left[(a-r\lambda)^2+r^2\xi^2+r^2\nu^2\right]^{1/2}} - \frac{1}{2}\Omega^2 \left[(r\lambda-\mu a)^2+r^2\xi^2\right] \tag{36}$$

where Ω is the Keplerian angular velocity is:

$$\Omega^2 = \frac{G\left(M_p + M_s\right)}{a^3}. \tag{37}$$

Note that for a fluid body with an isothermal atmosphere, surfaces of constant pressure coincide with surfaces of constant Roche potential. The appendix in Lindal et al. (1985) gives a numerical method for calculating surfaces of constant potential that can be adapted to any gravity field.

The Roche potential along the star-planet line is

$$\phi_R(r,\pi/2,0) = -\frac{GM_p}{r} - \frac{GM_s}{a-r} - \frac{1}{2}\Omega^2 (r-\mu a)^2 \tag{38}$$

and thus the gravity along this line is

$$g(r) = -\frac{GM_p}{r^2} + \frac{GM_s}{(a-r)^2} + \Omega^2 (r-\mu a). \tag{39}$$

The L1 point along the star-planet line is the vertex of the 'Roche lobe', which in turn is the last equipotential beyond which the equipotentials are open to infinity or encompass the star. At the L1 point, $g(r) = 0$, and we obtain the approximate location of the L1 point for small ratio M_p/M_s (Erkaev et al., 2007):

$$R_{L1} \approx \left(\frac{1}{3}\frac{M_p}{M_s}\right)^{1/3} a. \tag{40}$$

Erkaev et al. (2007) also derived an approximation for the potential difference between the surface of the planet and the L1 point along the planet-star line:

$$\Delta\phi_g = \phi_g(R_p)\left(1 - \frac{3}{2\xi} + \frac{1}{2\xi^3}\right) = \phi_g(R_p)K(\xi) \tag{41}$$

where $\xi = R_{L1}/R_p$. Since the L1 point lies on the Roche lobe, which is a surface of constant Roche potential, and because pressure levels line up approximately with surfaces of constant potential, this expression is valid for the potential difference between the surface and the Roche lobe at all latitudes and longitudes, provided that the surface (1 bar, R_p) can be approximated as spherical. Erkaev et al. (2007) go on to argue that escaping particles only need to overcome this potential difference, which is smaller than the difference between the surface and infinity for normal gravity, to be lost and contribute to the escape rate. Then the expression for energy-limited escape becomes

$$\dot{M}_E \approx \frac{\pi\epsilon F_{XUV} r_E^2}{\phi_g(R_p)K(\xi)}\left(\frac{R_s}{a}\right)^2 \tag{42}$$

where R_p is the surface radius of the planet at the substellar point.

This approximation is valid provided that the surface itself does not significantly deviate from spherical shape. A complete evaluation of $\Delta\phi_g$ starts from equation (36) and proceeds as follows: (i) calculate the Roche potential of the surface, by treating the transit radius as the polar radius, (ii) use the method of Lindal et al. (1985) or otherwise and the Roche potential to calculate the substellar radius at the surface, (iii) use the substellar radius to calculate gravity along the star-planet line and find the L1 point, (iv) calculate the potential difference between the L1 point and the surface, (v) insert this potential difference to the formula for energy-limited escape with Roche lobe effects. Note that even this approximation of the mass loss rate fails once the surface begins to approach the Roche lobe. Note also that the transit radius may not probe the 1 bar level, which may need to be taken into account for extremely close-in planets.

8.1 The Roche potential and Jeans escape

It is useful to observe that the thermal escape parameter can be adapted to any gravitational potential difference by writing it as

$$X = \frac{m\Delta\phi_g}{kT}, \tag{43}$$

which is correct for interpreting this parameter either in terms of the escape velocity V_{esc} or atmospheric structure. Technically, this allows us to adapt the formula for Jeans escape or modified Jeans escape to extremely close-in planets. Lecavelier des Etangs et al. (2004) used this approach and labeled it 'geometrical blow-off'. The planets for which this is relevant, however, would have to be significantly more massive than typical Hot Jupiters so that Jeans escape is valid in the first place.

9 The diffusion approximation

The momentum equation for neutral species s can be written as

$$\frac{\partial}{\partial t}(\rho_s w_s) + \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho_s w_s^2 r^2\right) + \frac{\partial p_s}{\partial r} + \rho_s g(r) = w_s \sum_t \rho_s R_{st} + \sum_{t \neq s} \rho_s \nu_{st}(w_t - w_s) \tag{44}$$

where the first term on the r.h.s describes momentum sources and sinks from chemical reactions and the second term, where ν_{st} is the momentum transfer collision frequency, describes collisions between species s and t. Assuming that $\rho_s w_s$ varies slowly over time and that the advection term (the second term on the l.h.s) and chemical reactions can be neglected, we have

$$\frac{\partial p_s}{\partial r} + \rho_s g(r) = \sum_{t \neq s} \rho_s \nu_{st}(w_t - w_s). \tag{45}$$

In hydrostatic equilibrium

$$g(r) = -\frac{1}{\rho}\frac{\partial p}{\partial r}$$

and thus

$$\frac{\partial p_s}{\partial r} - \frac{\rho_s}{\rho}\frac{\partial p}{\partial r} = \sum_{t\neq s} \rho_s \nu_{st} (w_t - w_s). \tag{46}$$

We write the partial pressure gradient in terms of the volume mixing ratio $x_s = n_s/n$ as

$$\frac{\partial p_s}{\partial r} = p\frac{\partial x_s}{\partial r} + x_s\frac{\partial p}{\partial r}, \tag{47}$$

which gives the diffusion approximation for the gradient of the mixing ratio x_s as

$$\frac{\partial x_s}{\partial r} + \left(x_s - \frac{\rho_s}{\rho}\right)\frac{1}{p}\frac{\partial p}{\partial r} = -\sum_{t\neq s} x_s x_t \frac{w_s - w_t}{D_{st}} \tag{48}$$

where

$$D_{st} = \frac{x_t kT}{m_s \nu_{st}} \tag{49}$$

is the mutual diffusion coefficient.

10 Diffusion-limited escape

Diffusion-limited flux (Hunten, 1973) is the maximum escape flux of a minor, lighter species escaping from an atmosphere dominated by a major, heavier species ($m_s < m$). We derive the basic form by assuming that the background atmosphere is stationary and that mixing of the atmosphere by turbulence, breaking waves and circulation is parameterized by an eddy diffusion coefficient K_{zz} so that

$$\frac{\partial x_s}{\partial r} + \left(x_s - \frac{\rho_s}{\rho}\right)\frac{1}{p}\frac{\partial p}{\partial r} = -\sum_{t\neq s} x_s x_t \frac{w_s - w_K}{D_{st}} \tag{50}$$

where

$$w_K = -K_{zz}\frac{1}{x_s}\frac{\partial x_s}{\partial r} \tag{51}$$

and thus

$$\frac{\partial x_s}{\partial r} + \left(x_s - \frac{\rho_s}{\rho}\right)\frac{1}{p}\frac{\partial p}{\partial r} = -\sum_{t\neq s} x_s x_t \frac{1}{D_{st}}\left(w_s + K_{zz}\frac{1}{x_s}\frac{\partial x_s}{\partial r}\right). \tag{52}$$

We define the diffusion coefficient for species s as

$$\frac{1}{D_s} = \sum_{t\neq s}\frac{x_t}{D_{st}} \tag{53}$$

and obtain

$$\frac{D_s+K_{zz}}{D_s}\frac{\partial x_s}{\partial r}+\left(x_s-\frac{\rho_s}{\rho}\right)\frac{1}{p}\frac{\partial p}{\partial r}=-\frac{x_s w_s}{D_s}, \tag{54}$$

which gives us the flux

$$f_s = n_s w_s = \frac{n_s D_s}{H}\left(1-\frac{m_s}{m}\right)-n\left(D_s+K_{zz}\right)\frac{\partial x_s}{\partial r} \tag{55}$$

where H is the pressure scale height.

The diffusion-limited flux f_L is defined as

$$f_L \equiv \frac{n_s D_s}{H}\left(1-\frac{m_s}{m}\right) \tag{56}$$

so that

$$\frac{\partial x_s}{\partial r}=\frac{1}{n\left(D_s+K_{zz}\right)}\left(f_L-f_s\right). \tag{57}$$

If $f_s < f_L$, the gradient of the mixing ratio positive and the mixing ratio increases with altitude, which is the expected behavior for a lighter minor species. If $f_s = f_L$, the gradient is constant and the atmosphere is well mixed – this is the maximum possible escape flux for the minor species. Fluxes higher than this lead to a negative mixing ratio gradient and choke off the flow until the system returns to $f_s = f_L$ and constant mixing ratio with radius.

11 Escape of minor heavy species: Cross-over mass

Hunten et al. (1987) derived the concept of the cross-over mass to describe mass fractionation in hydrodynamic escape and its possible impact on the early atmospheres of Venus, Earth and Mars. The cross-over mass is the maximum mass m_c of a minor species that can 'carried out' by a major lighter species and escape the atmosphere. Assuming that $K_{zz} << D_s$ (see below), we write equation (50) for two species, focusing on the background minor species 2:

$$\begin{aligned}\frac{1}{x_2}\frac{\partial x_2}{\partial r} &= \frac{mg}{kT}-\frac{m_2 g}{kT}+\frac{1}{nD_{12}}\left(f_1-\frac{x_1}{x_2}f_2\right)\\ &= \frac{1}{nD_{12}}\left(f_1-\frac{x_1}{x_2}f_2\right)-\left(m_2-m_1\right)\frac{x_1 g}{kT}\end{aligned} \tag{58}$$

where the mean molecular weight is $m = x_1m_1 + x_2m_2$, $f_1 = n_1w_1$ and $x_2 - 1 = -x_1$. Here we assumed that $T_1 = T_2$ and, perhaps most importantly, that

$$\frac{1}{p}\frac{\partial p}{\partial r}=-\frac{mg}{kT}, \tag{59}$$

which, interestingly, is technically invalid for hydrodynamic escape.

Assume that the mixing ratio of the minor heavy species 2 is constant with altitude due to drag forces from species 1. In this case the right hand side of equation (58) is zero and we have

$$f_2 = \frac{x_2}{x_1} f_1 \left[1 - \frac{nD_{12}x_1 g}{kT f_1} (m_2 - m_1) \right] . \tag{60}$$

For physical solutions we require that $f_2 \geq 0$ and thus we insist that

$$\frac{nD_{12}x_1 g}{kT f_1} (m_2 - m_1) \leq 1 \rightarrow m_2 \leq m_c = m_1 + \frac{kT f_1}{nD_{12} g x_1} \tag{61}$$

where m_c is the cross-over mass. When $m_2 > m_c$, f_2 goes negative and the condition that the mixing ratio of species 2 is constant with altitude is no longer satisfied - in this case diffusive separation sets in. Note that one could bring K_{zz} into this formulation but this would make no difference as D_{12} becomes much larger than K_{zz} at high altitudes where x_2 is still constant with altitude as long as $m_2 < m_c$.

Koskinen et al. (2014) used this formulation to derive the minimum mass loss rate of the lighter major species 1 that is required to drag a heavier minor species 2 out of the atmosphere. In this case we have

$$f_1 \geq \frac{nD_{12}x_1 g}{kT} (m_2 - m_1) \rightarrow \dot{M}_1 \geq 4\pi m_1 G M_p (m_2 - m_1) \frac{nD_{12}}{kT} \tag{62}$$

where $\dot{M} = 4\pi r^2 m_1 f_1$ and we used $g = GM_p/r^2$ where M_p is the planet mass. Note that this formula does not depend on altitude for an isothermal atmosphere because

$$\frac{nD_{12}}{T} = \frac{n_2 k}{m_1 \nu_{12}} \tag{63}$$

where ν_{12} is proportional to n_2 and $f_1 r^2$ is constant with altitude.

References

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