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Steady solution of the Boltzmann equation for evaporation and condensation on a planar interface with a general boundary condition

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Abstract

The half-space problem for steady gas flow with evaporation or condensation is studied for the case where the gas–liquid interaction law, i.e., the kinetic boundary condition at the gas–liquid interface, is extended to a wide class. It is shown that the half-space problem can be formulated as independent of the detail of the generalized kinetic boundary condition concerned. On the basis of this fact, we show that the steady solution of Boltzmann equation with the generalized kinetic boundary condition can be obtained from the steady solution for the complete condensation condition.

1 Introduction

It is well known that the gas behavior near the boundary is essentially in a nonequilibrium state unless the entire flow field is in a equilibrium state. The typical length scale characterizing the nonequilibrium behavior of gas near the boundary is the mean free path of the gas molecules, ℓ, and the nonequilibrium region is called the Knudsen layer, if the characteristic length scale for the entire flow field, say L, is sufficiently large compared with the mean free path ℓ. The gas behavior outside the Knudsen layer may be regarded in a local equilibrium state in the leading order of approximation, and hence the gas behavior can be determined by the macroscopic quantities, such as the gas density, gas velocity, gas temperature, and so on, and the macroscopic quantities are governed by equations of fluid mechanics.

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In the presence of evaporation or condensation at the vapor–liquid interface, the gas near the gas–liquid interface cannot be in an equilibrium state. Therefore, the boundary conditions for fluid mechanics equations should be derived from the kinetic theory of gases or the molecular gas dynamics. To do so, we have to solve the Boltzmann equation with the kinetic boundary condition at the gas–liquid interface and the boundary condition at a distant region where the gas is in a local equilibrium state. This is called the half-space problem of gas flow with evaporation or condensation.

The half-space problem has been extensively studied by Sone and his colleagues (Sone 1978, Sone & Onishi 1978, Sone, Aoki & Yamashita 1986, Sone, Aoki, Sugimoto & Yamada 1988, Sone & Sugimoto 1990, Aoki, Sone & Yamada 1990, Aoki, Nishino, Sone & Sugimoto 1991, Sone, Aoki & Doi 1992, Sone, Golse, Ohwada & Doi 1998, Bardos, Golse & Sone 2006). Most of above studies have treated the case of kinetic boundary condition of complete condensation type; the case of a generalized boundary condition has been discussed by Aoki & Sone (1991) and Sone (2006).

In the present paper, we address a further generalized boundary condition, in which the velocity distribution function for the molecules leaving the interface is assumed to be a half of Maxwellian multiplied by a factor $\mathcal{A}$, and we don't require any special property for $\mathcal{A}$. We have proposed this type of kinetic boundary condition at the interface through a series of molecular dynamics studies (Ishiyama, Yano & Fujikawa 2004a, Ishiyama, Yano & Fujikawa 2004b, Ishiyama, Yano & Fujikawa 2005).

2 Governing equation and boundary condition

Consider the semi-infinite space filled with a condensable monatomic gas and bounded by a planar condensed phase of the same molecules. The temperature of the condensed phase is T_w, which is constant, and the gas at a distant region from the condense phase is in an equilibrium state.

We assume that the gas is an ideal gas and its behavior is independent of time and the space coordinates parallel to the interface of gas and condensed phase. Then, the gas behavior is governed by the Boltzmann equation

$$\xi_1 \frac{\partial f}{\partial X_1} = J(f,f), \quad (0 < X_1 < \infty), \tag{1}$$

where $f(X_1, \xi_i)$ is the velocity distribution function of gas molecule, ξ_i ($i = 1,2,3$) is the molecular velocity, X_1 is the space coordinate, the subscript 1 denotes the component normal to the interface, and the interface is located at $X_1 = 0$. The right-hand side of Eq. (1), $J(f,f)$, is the collision term that describes the binary collision of gas molecules. We don't mention the detail of the collision term for a while and in fact the present theory is not restricted to any specific form of collision term.

A generalized kinetic boundary condition that we study here is

$$f = \frac{\mathcal{A}}{(2\pi RT_w)^{3/2}} \exp\left(-\frac{\xi_i^2}{2RT_w}\right), \quad (X_1 = 0,\ \xi_1 > 0), \tag{2}$$

where R is the gas constant. Here, we assume (i) $\mathcal{A} > 0$, (ii) $\mathcal{A}$ is a function of T_w, (iii) $\mathcal{A}$ is independent of ξ_i.

If $\mathcal{A} = \rho^*$, where ρ^* is the saturated vapor density at temperature T_w, then Eq. (2) reduces to the complete condensation condition, the case of which has been extensively studied by Sone and his colleagues. If $\mathcal{A} = \alpha\rho^* + (1-\alpha)\sigma$, then Eq. (2) reduces to the boundary condition discussed by Aoki & Sone (1991) and Sone (2006), where α is a constant $(0 < \alpha < 1)$ specified in advance. The mass flux of the molecules incident on the interface is represented by σ, defined by

$$\sigma = -\left(\frac{2\pi}{RT_w}\right)^{1/2} \int_{\xi_1<0} \xi_1 f\Big|_{X_1=0} \mathbf{d}\boldsymbol{\xi}, \tag{3}$$

where $\mathbf{d}\boldsymbol{\xi} = d\xi_1 d\xi_2 d\xi_3$ and the range of integration is $-\infty < \xi_1 < 0$ and $-\infty < \xi_1, \xi_2 < \infty$; if nothing is stated, the integration is carried out over the whole space of ξ_i. In the latter case, $\mathcal{A}$ is dependent on f for $\xi_1 < 0$ at $X_1 = 0$ through σ. This does not conflict with the above three assumptions on $\mathcal{A}$.

We shall remark that if $\mathcal{A} \neq \rho^*$, $\mathcal{A}$ should depend on f for $\xi_1 < 0$ at $X_1 = 0$ so that the equilibrium state at T_w can be satisfied by Eq. (2). In this case, the numerical value of $\mathcal{A}$ cannot be specified before solving the problem, as in the case of $\mathcal{A} = \alpha\rho^* + (1-\alpha)\sigma$.

The boundary condition at infinity is given by

$$f = \frac{\rho_\infty}{(2\pi RT_\infty)^{3/2}} \exp\left[-\frac{(\xi_i - v_\infty)^2}{2RT_\infty}\right], \quad (X_1 \to \infty), \tag{4}$$

where ρ_∞, $v_{i\infty}$, and T_∞ are, respectively, the gas density, the gas velocity, and the gas temperature at infinity, which are constants and $v_{2\infty} = v_{3\infty} = 0$. Aoki, Nishino, Sone & Sugimoto (1991) have extended the half-space problem to the case where $v_{2\infty} \neq 0$.

3 Reformulation of the half-space problem

3.1 Nondimensionalization

The half-space problem (1)(2)(4) can be nondimensionalized as follows:

$$\zeta_1 \frac{\partial \hat{f}}{\partial x_1} = \frac{2}{\sqrt{\pi}} \hat{J}(\hat{f}, \hat{f}), \quad (0 < x_1 < \infty), \tag{5}$$

$$\hat{f} = \frac{\hat{A}}{\pi^{3/2}} e^{-\zeta_i^2}, \quad (x_1 = 0, \zeta_1 > 0), \tag{6}$$

$$\hat{f} = \frac{\hat{\rho}_\infty}{(\pi \hat{T}_\infty)^{3/2}} \exp\left[- \frac{(\zeta_i - \hat{v}_{i\infty})^2}{\hat{T}_\infty} \right], \quad (x_1 \to \infty). \tag{7}$$

The nondimensional variables are defined as

$$x_1 = \frac{X_1}{\ell_0}, \quad \zeta_i = \frac{\xi_i}{\sqrt{2RT_w}}, \quad \hat{f} = \frac{f(2RT_w)^{3/2}}{\rho^*}, \quad \hat{A} = \frac{A}{\rho^*}, \tag{8}$$

$$\hat{\rho}_\infty = \frac{\rho_\infty}{\rho^*}, \quad \hat{v}_{i\infty} = \frac{v_{i\infty}}{\sqrt{2RT_w}}, \quad \hat{T}_\infty = \frac{T_\infty}{T_w}, \tag{9}$$

where ℓ_0 is the mean free math in the equilibrium state at temperature T_w and density ρ^*.

3.2 Mass flux across the interface

The mass flux across the interface, m, is given by

$$m = \int \xi_1 f \Big|_{X_1=0} \mathbf{d\xi} = \rho_\infty v_{1\infty}, \tag{10}$$

where the first equal sign is the definition and the second sign holds because of the assumption of steady state. Substituting the definitions of nondimensional variables into Eq. (10) leads to the nondimensional relation for mass flux across the interface,

$$\hat{m} = \hat{\rho}_\infty \hat{v}_{1\infty} = \int_{\zeta_1 > 0} \zeta_1 \hat{f} \Big|_{x_1=0} \mathbf{d\zeta} + \int_{\zeta_1 < 0} \zeta_1 \hat{f} \Big|_{x_1=0} \mathbf{d\zeta} = \frac{\hat{A} - \hat{\sigma}}{2\sqrt{\pi}}, \tag{11}$$

where $\mathbf{d\zeta} = \mathrm{d}\zeta_1 \mathrm{d}\zeta_2 \mathrm{d}\zeta_3$ and

$$\hat{\sigma} = -2\sqrt{\pi} \int_{\zeta_1 < 0} \zeta_1 \hat{f} \Big|_{x_1=0} \mathbf{d\zeta}. \tag{12}$$

Making use of Eq. (11), we can eliminate $\mathcal{A}$ from the nondimensional kinetic boundary condition at the interface, Eq. (6), and we have

$$\hat{f} = \frac{2\sqrt{\pi}\hat{\rho}_\infty \hat{v}_{1\infty} + \hat{\sigma}}{\pi^{3/2}} e^{-\zeta_i^2}, \quad (x_1 = 0,\, \zeta_1 > 0), \tag{13}$$

That is, the half-space problem (1)(2)(4) can be formulated as Eqs. (5), (13), and (7), irrespective of $\mathcal{A}$, i.e., the detail of gas–liquid interaction law.

3.3 Elimination of $\hat{\rho}_\infty$

Introducing new variables

$$\bar{f} = \frac{\hat{f}}{\hat{\rho}_\infty}, \quad \bar{x}_1 = \hat{\rho}_\infty x_1, \quad \bar{\sigma} = \frac{\hat{\sigma}}{\hat{\rho}_\infty} = -2\sqrt{\pi}\int_{\zeta_1<0} \zeta_1 \bar{f}\Big|_{x_1=0} \mathrm{d}\boldsymbol{\zeta}, \tag{14}$$

we can transform the half-space problem, Eqs. (5), (13), and (7), into

$$\zeta_1 \frac{\partial \bar{f}}{\partial \bar{x}_1} = \frac{2}{\sqrt{\pi}} \hat{J}(\bar{f}, \bar{f}), \quad (0 < \bar{x}_1 < \infty), \tag{15}$$

$$\bar{f} = \frac{2\sqrt{\pi}\hat{v}_{1\infty} + \bar{\sigma}}{\pi^{3/2}} e^{-\zeta_i^2}, \quad (\bar{x}_1 = 0,\, \zeta_1 > 0), \tag{16}$$

$$\bar{f} = \frac{1}{(\pi \hat{T}_\infty)^{3/2}} \exp\left[-\frac{(\zeta_i - \hat{v}_{i\infty})^2}{\hat{T}_\infty} \right], \quad (\bar{x}_1 \to \infty). \tag{17}$$

It is clear that the half-space problem (15)(16)(17) is independent of $\hat{\rho}_\infty$ and hence its solution $\bar{f}$ is also independent of $\hat{\rho}_\infty$. If we could solve the half-space problem (15)(16)(17) and obtain $\bar{f}$ as a function of $\bar{x}_1$ and ζ_i, the solution $\hat{f}$ of the half-space problem, Eqs. (5), (13), and (7), would be retrieved by a conversion formula

$$\hat{f}(x_1, \zeta_i; \hat{\rho}_\infty, \hat{v}_{1\infty}, \hat{T}_\infty) = \hat{\rho}_\infty \bar{f}(\hat{\rho}_\infty \bar{x}_1, \zeta_i; \hat{v}_{1\infty}, \hat{T}_\infty). \tag{18}$$

3.4 Existence of solution

What is of importance in the half-space problem (5)(6)(7) is the existence of a set $(\hat{\rho}_\infty, \hat{v}_{1\infty}, \hat{T}_\infty)$ that allows the half-space problem to have a solution. Such a set $(\hat{\rho}_\infty, \hat{v}_{1\infty}, \hat{T}_\infty)$ is used as the boundary condition for fluid mechanics equations outside the Knudsen layer.

The mathematical proof of the existence of a set $(\hat{\rho}_\infty, \hat{v}_{1\infty}, \hat{T}_\infty)$ that allows the half-space problem to have a solution or the existence of the solution of the half-space problem seems not to be obtained. However, as long as the case of the complete condensation condition, the extensive numerical study by Sone and his colleagues has been accepted as a numerical proof.

As mentioned above, the complete condensation condition is prescribed by $\hat{\mathcal{A}} = 1$ and hence the mass flux relation (11) can be written as

$$2\sqrt{\pi}\hat{v}_{1\infty} + \bar{\sigma} = \frac{1}{\hat{\rho}_\infty}. \tag{19}$$

Since the existence of the solution of the half-space problem, Eqs. (5), (13), and (7) with Eq. (19), has been proved numerically, the solution $\hat{f}(x_1, \zeta_i)$ exists for some set $(\hat{\rho}_{\infty C}, \hat{v}_{1\infty C}, \hat{T}_{\infty C})$, where the subscript C denotes the set that allows the half-space problem to have a solution for the complete condensation condition. The solution $\bar{f}(\bar{x}_1, \zeta_i)$ for the half-space problem (15)(16)(17) with Eq. (19) is then obtained by using the conversion formula (18) inversely.

For $\hat{\mathcal{A}} \neq 1$, the mass flux relation (11) can be written as

$$2\sqrt{\pi}\hat{v}_{1\infty} + \bar{\sigma} = \frac{1}{\hat{\rho}_\infty/\hat{\mathcal{A}}}. \tag{20}$$

Therefore, the solution of the half-space problem (15)(16)(17) actually exists for the set $(\hat{\rho}_\infty, \hat{v}_{1\infty}, \hat{T}_\infty) = (\hat{\rho}_{\infty C}\hat{\mathcal{A}}, \hat{v}_{1\infty C}, \hat{T}_{\infty C})$, and it is substantially equivalent to the solution for the complete condensation condition. In fact, making use of the fact that $\bar{f}_{\hat{\mathcal{A}}\neq 1} = \bar{f}_{\hat{\mathcal{A}}=1}$ and

$$\hat{\rho}_\infty \bar{f}_{\hat{\mathcal{A}}\neq 1}(\hat{\rho}_\infty \bar{x}_1, \zeta_i) = \hat{f}_{\hat{\mathcal{A}}\neq 1}(x_1, \zeta_i), \quad \frac{\hat{\rho}_\infty}{\hat{\mathcal{A}}}\bar{f}_{\hat{\mathcal{A}}=1}\left(\frac{\hat{\rho}_\infty}{\hat{\mathcal{A}}}\bar{x}_1, \zeta_i\right) = \hat{f}_{\hat{\mathcal{A}}=1}(x_1, \zeta_i), \tag{21}$$

we immediately have

$$\hat{f}_{\hat{\mathcal{A}}\neq 1}(x_1, \zeta_i) = \hat{\mathcal{A}}\hat{f}_{\hat{\mathcal{A}}=1}(\hat{\mathcal{A}}x_1, \zeta_i) \tag{22}$$

where the subscripts $\hat{\mathcal{A}} \neq 1$ and $\hat{\mathcal{A}} = 1$ represent the solutions for $\hat{\mathcal{A}} \neq 1$ and $\hat{\mathcal{A}} = 1$, respectively.

4 Numerical example

Here, we confine ourselves to subsonic evaporation or subsonic condensation state and we employ the Boltzmann–Krook–Welander (BKW) equation (Sone 2006). The finite-difference method is used after the elimination of ζ_2 and ζ_3 from the BKW equation, the methodology of which has been widely known (Sone, Aoki & Yamashita 1986, Sone & Sugimoto 1990, Aoki, Sone & Yamada 1990, Aoki, Nishino, Sone & Sugimoto 1991, Sone 2006). Sone and his colleagues have summarized their results in terms of p_∞/p_w, T_∞/T_w,

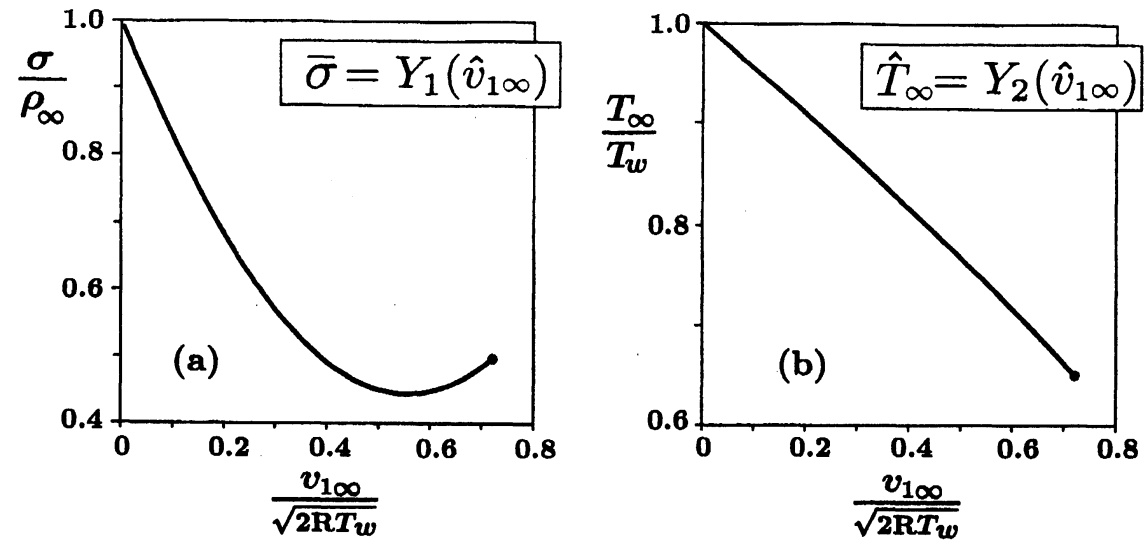

Fig. 1. Numerical results for subsonic evaporation. (a) The relation between $\bar{\sigma}$ and $\hat{v}_{1\infty}$. (b) The relation between $\hat{T}_\infty$ and $\hat{v}_{1\infty}$.

and $v_{1\infty}/[(5/3)RT_\infty]^{1/2}$ (and velocity component tangential to the interface). In the following, however, since $\hat{\rho}_\infty$ is eliminated in the half-space problem (15)(16)(17), it is sufficient to explore the two-dimensional parameter plane $(\hat{v}_{1\infty}, \hat{T}_\infty)$.

4.1 Subsonic evaporation

In Fig. 1, we plot the numerically obtained functions $\bar{\sigma} = Y_1(\hat{v}_{1\infty})$ and $\hat{T}_\infty = Y_2(\hat{v}_{1\infty})$ for subsonic evaporation. The black spot in the figure designates the sonic limit. The subsonic evaporation state is simply determined by $\hat{v}_\infty$ through functions Y_1 and Y_2, which correspond to h_1 and h_2 functions tarbulated in the book by Sone (2006).

4.2 Subsonic condensation

Figure 2 shows the numerically obtained function $\bar{\sigma} = Y_3(\hat{v}_{1\infty}, \hat{T}_\infty)$. The black spot in the figure designates the sonic limit. The Y_3 function corresponds to the F_s function in the book by Sone (2006).

4.3 Temperature jump

In Fig. 3, the gas temperature $T_{\rm B}$ divided by the temperature of the interface T_w is shown as a function of $\hat{T}_\infty$ and $\hat{v}_{1\infty}$ for subsonic condensation (Fig. 3(a))

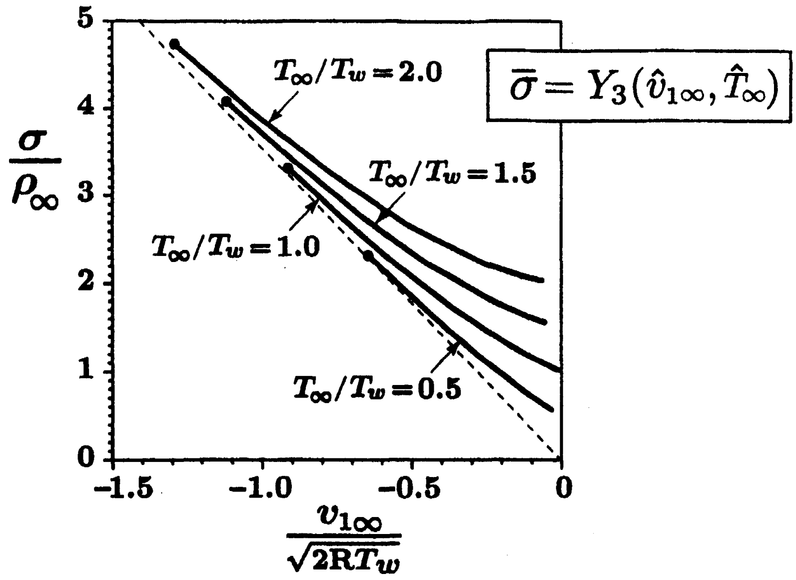

Fig. 2. Numerical results for subsonic evaporation. The $\bar{\sigma}$ is plotted as a function of $\hat{v}_{1\infty}$ and $\hat{T}_\infty$.

and as a function of $\hat{v}_{1\infty}$ for subsonic evaporation (Fig. 3(b)). The difference between T_B and T_w is called the temperature jump.

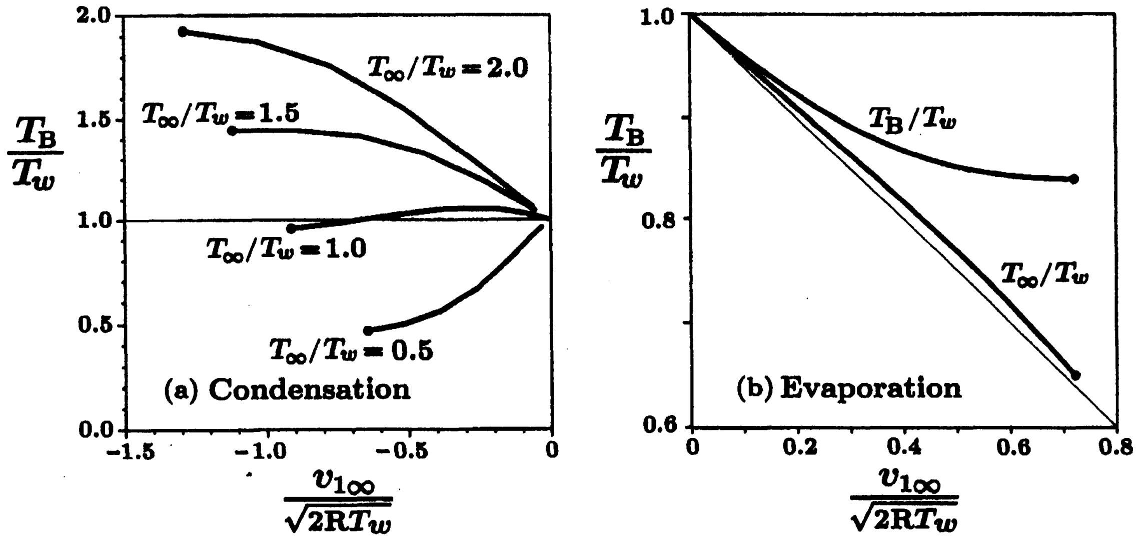

Fig. 3. The gas temperature at the interface T_B. (a) Subsonic condensation. (b) Subsonic evaporation.

5 Conclusion

The half-space problem of the gas flow with evaporaion or condensation has been considered for the case that the kinetic boundary condition at the interface between the gas and its condensed phase is generalized. We have eliminated $\mathcal{A}$ and ρ_∞ from the formulation of the problem, and thereby demonstrating that the solution of the half-space problem (15)(16)(17) actually exists for the set $(\hat{\rho}_\infty, \hat{v}_{1\infty}, \hat{T}_\infty) = (\hat{\rho}_{\infty C}\hat{\mathcal{A}}, \hat{v}_{1\infty C}, \hat{T}_{\infty C})$, and it is substantially equivalent to the solution for the complete condensation condition.

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