

# Relaxation Phenomena of Binary Gas-Mixture with Sizable Difference in their Temperatures and Velocities on the basis of Boltzmann Equations

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**Abstract.** Relaxation phenomena in the binary gas-mixture with different temperature and different velocities are discussed on the basis of two Boltzmann equations. The Hermite expansion method, extended by H.Grad to multi-dimensional space, is applied to express distribution functions and the Galerkin method is used to solve two Boltzmann equations. Thus, a system of differential equations for the expansion coefficients is obtained. The time development of the system is calculated numerically.

**Keywords:** Relaxation, Gas-Mixture, Hermite Expansion, Boltzmann Equations.

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## INTRODUCTION

Relaxation phenomena in the binary gas-mixture with different temperatures and different velocities are discussed on the basis of two Boltzmann equations. The separate heating of the binary gas-mixture could be done, for example, by hydrogen gas and water vapor in a glass container in a microwave oven. The microwave oven is devised as stronger heating of water than the hydrogen gas. The electric current in plasma would be an example of different velocities. The Hermite expansion method of the distribution function is developed by H. Grad<sup>1</sup> for solving Boltzmann equation of a simple gas. This method would be extended to binary gas-mixture, *i.e.* the Hermite expansion to two distribution functions for both gases is taken. We have two Boltzmann equations expanded by Hermite functions. The Galerkin method is applied to solve two Boltzmann equations, *i.e.* the scalar products of Hermite functions and the Boltzmann equations are taken. Thus, a system of partial differential equations for the expansion coefficients is obtained and the coefficients are functions of position and time. We calculate numerically the time development of the solutions.

## BASIC EQUATIONS

We have the Boltzmann equations for two gases:

$$\begin{aligned} B(f^{(i)}, f^{(j)}) &\equiv \frac{\partial f^{(i)}}{\partial t} + (\tilde{\mathbf{c}}^{(i)} + \mathbf{v}^{(i)}) \cdot \frac{\partial f^{(i)}}{\partial \mathbf{x}} - \left( \frac{\partial \mathbf{v}^{(i)}}{\partial t} + \mathbf{v}^{(i)} \cdot \frac{\partial \mathbf{v}^{(i)}}{\partial \mathbf{x}} \right) \cdot \frac{\partial f^{(i)}}{\partial \tilde{\mathbf{c}}^{(i)}} - \left( \left( \tilde{\mathbf{c}}^{(i)} \cdot \frac{\partial}{\partial \mathbf{x}} \right) \mathbf{v}^{(i)} \right) \cdot \frac{\partial f^{(i)}}{\partial \tilde{\mathbf{c}}^{(i)}} - J^{(i)} - J^{(j)} = 0, \\ J^{(j)} &= \iiint \iint \left\{ f^{(i)}(\mathbf{x}, \tilde{\mathbf{c}}^{(i)}, t) f^{(j)}(\mathbf{x}, \tilde{\mathbf{c}}^{(j)}, t) - f^{(i)}(\mathbf{x}, \tilde{\mathbf{c}}^{(i)}, t) f(\mathbf{x}, \tilde{\mathbf{c}}^{(j)}, t) \right\} k_c^{(ij)}(\mathbf{b}^{(ij)}, |\mathbf{c}^{(j)} - \mathbf{c}^{(i)}|) d^2 \mathbf{k} d^3 \tilde{\mathbf{c}}^{(j)}, \end{aligned} \quad (1)$$

where  $m^{(i)}$ ,  $\mathbf{v}^{(i)}(\mathbf{x}, t)$  and  $\tilde{\mathbf{c}}^{(i)}(\mathbf{x}, \mathbf{c}^{(i)}, t) = \mathbf{c}^{(i)} - \mathbf{v}^{(i)}(\mathbf{x}, t)$  are respectively the mass, the mean velocity and the peculiar velocity of the  $i$ -molecule.  $k_c^{(ij)}$  can be written as

$$k_c^{(ij)}(\mathbf{b}^{(ij)}, |\mathbf{c}^{(j)} - \mathbf{c}^{(i)}|) = |\mathbf{c}^{(j)} - \mathbf{c}^{(i)}| \frac{b^{(ij)}}{\sin \chi^{(ij)}} \left| \frac{\partial b^{(ij)}}{\partial \chi^{(ij)}} \right|, \quad (2)$$

where  $b^{(ij)}$  and  $\chi^{(ij)}$  are the collision parameter and the deflection angle between  $i$ - and  $j$ -molecules. Furthermore, the molecular velocities of the final state are

$$\mathbf{c}^{(i')} = \tilde{\mathbf{c}}^{(i)} + \frac{2m^{(j)}}{m^{(i)} + m^{(j)}} \left( (\tilde{\mathbf{c}}^{(j)} - \tilde{\mathbf{c}}^{(i)} + \mathbf{v}^{(j)} - \mathbf{v}^{(i)}) \cdot \mathbf{k} \right) \mathbf{k}, \quad \tilde{\mathbf{c}}^{(j')} = \tilde{\mathbf{c}}^{(j)} - \frac{2m^{(i)}}{m^{(i)} + m^{(j)}} \left( (\tilde{\mathbf{c}}^{(j)} - \tilde{\mathbf{c}}^{(i)} + \mathbf{v}^{(j)} - \mathbf{v}^{(i)}) \cdot \mathbf{k} \right) \mathbf{k}. \quad (3)$$

The collision term is valid for  $j = i$ . The macroscopic physical values, that is, number density, mean velocity, temperature, pressure, pressure tensor, heat flow and the internal energy are defined respectively as follows,

$$\left. \begin{aligned} n^{(i)}(\mathbf{x}, t) &= \int f^{(i)}(\mathbf{c}^{(i)}, \mathbf{x}, t) d\mathbf{c}^{(i)}, \\ \mathbf{v}^{(i)}(\mathbf{x}, t) &= \frac{1}{n^{(i)}(\mathbf{x}, t)} \int \mathbf{c}^{(i)} f^{(i)}(\mathbf{c}^{(i)}, \mathbf{x}, t) d\mathbf{c}^{(i)}, \\ T^{(i)}(\mathbf{x}, t) &= \frac{m^{(i)}}{3k_B n^{(i)}(\mathbf{x}, t)} \int (\mathbf{c}^{(i)} - \mathbf{v}^{(i)}(\mathbf{x}, t))^2 f^{(i)}(\mathbf{c}^{(i)}, \mathbf{x}, t) d\mathbf{c}^{(i)}, \\ p^{(i)}(\mathbf{x}, t) &= \frac{1}{3} \int m^{(i)} (\mathbf{c}^{(i)} - \mathbf{v}^{(i)}(\mathbf{x}, t))^2 f^{(i)}(\mathbf{c}^{(i)}, \mathbf{x}, t) d\mathbf{c}^{(i)}, \\ p_{\mu\nu}^{(i)}(\mathbf{x}, t) &= \int m^{(i)} (c_\mu^{(i)} - v_\mu^{(i)}(\mathbf{x}, t)) (c_\nu^{(i)} - v_\nu^{(i)}(\mathbf{x}, t)) f^{(i)}(\mathbf{c}^{(i)}, \mathbf{x}, t) d\mathbf{c}^{(i)}, \\ q_\mu^{(i)}(\mathbf{x}, t) &= \frac{N^{(i)}}{3} \int \frac{1}{2} m^{(i)} (c_\mu^{(i)} - v_\mu^{(i)}(\mathbf{x}, t)) (\mathbf{c}^{(i)} - \mathbf{v}^{(i)})^2 f^{(i)}(\mathbf{c}^{(i)}, \mathbf{x}, t) d\mathbf{c}^{(i)}, \\ e^{(i)}(\mathbf{x}, t) &= \frac{(3 + N^{(i)})}{2m^{(i)}} n^{(i)}(\mathbf{x}, t) k_B T^{(i)}(\mathbf{x}, t) \end{aligned} \right\} \quad (4)$$

Where  $N^{(i)}$  is the degree of freedom of the translational and internal motions in a molecule.

## HERMITE EXPANSION

The Hermite expansion method developed by H.Grad for solving Boltzmann equation for a simple gas, would be extended to binary gas-mixture. The Hermite functions are defined as follows,

$$\begin{aligned} H_0^{(0)}(\boldsymbol{\xi}^{(i)}) &= 1, \quad H_\lambda^{(1)}(\boldsymbol{\xi}^{(i)}) = \xi_\lambda^{(i)}, \quad H_{\lambda\mu}^{(2)}(\boldsymbol{\xi}^{(i)}) = \xi_\lambda^{(i)} \xi_\mu^{(i)} - \delta_{\lambda\mu} \\ H_{\lambda\mu\nu}^{(3)}(\boldsymbol{\xi}^{(i)}) &= \xi_\lambda^{(i)} \xi_\mu^{(i)} \xi_\nu^{(i)} - (\xi_\lambda^{(i)} \delta_{\mu\nu} + \xi_\mu^{(i)} \delta_{\nu\lambda} + \xi_\nu^{(i)} \delta_{\lambda\mu}), \quad (1 \leq \lambda, \mu \leq 3) \quad \text{etc} \end{aligned} \quad (5)$$

Where,  $\boldsymbol{\xi}^{(i)}$  is normalized peculiar velocity and the parameter  $\alpha^{(i)-1}$  is the thermal velocity as follows

$$\boldsymbol{\xi}^{(i)} = (\xi_1^{(i)}, \xi_2^{(i)}, \xi_3^{(i)}), \quad \boldsymbol{\xi}^{(i)} = \alpha^{(i)} \tilde{\mathbf{c}}^{(i)}, \quad \alpha^{(i)} = \sqrt{\frac{m^{(i)}}{k_B T^{(i)}(\mathbf{x}, t)}}. \quad (6)$$

Here, the velocity distribution function could be constructed as the product of the Maxwell distribution function and Hermite expansion. The rest is expressed by  $\varphi^{(i)}(\mathbf{x}, \boldsymbol{\xi}^{(i)}, t)$  which is generally described by the Hermite expansion as

$$\left. \begin{aligned} f^{(i)}(\mathbf{x}, \boldsymbol{\xi}^{(i)}, t) &= f_M^{(i)}(\mathbf{x}, \boldsymbol{\xi}^{(i)}, t) \phi^{(i)}(\mathbf{x}, \boldsymbol{\xi}^{(i)}, t) \\ f_M^{(i)}(\mathbf{x}, \boldsymbol{\xi}^{(i)}, t) &= n^{(i)}(\mathbf{x}, t) \left( \frac{\alpha^{(i)}}{\sqrt{2\pi}} \right)^3 e^{-\frac{1}{2} \boldsymbol{\xi}^{(i)2}} \\ \phi^{(i)}(\mathbf{x}, \boldsymbol{\xi}^{(i)}, t) &= \sum_{m=0}^{\infty} \left\{ \sum_{\ell_1=1}^3 \sum_{\ell_2=\ell_1}^3 \cdots \sum_{\ell_m=\ell_{m-1}}^3 A_{[\ell_m]}^{(i)}(\mathbf{x}, t) H_{[\ell_m]}^{(m)}(\boldsymbol{\xi}^{(i)}) \right\}, \quad [\ell_m] = \ell_0 \ell_1 \cdots \ell_m \end{aligned} \right\} \quad (7)$$

Then the distribution functions are described as

$$f^{(i)}(\mathbf{x}, \boldsymbol{\xi}^{(i)}, t) = f_M^{(i)}(\mathbf{x}, \boldsymbol{\xi}^{(i)}, t) \left\{ A_0^{(i)}(\mathbf{x}, t) + \sum_{\lambda=1}^3 A_\lambda^{(i)}(\mathbf{x}, t) H_\lambda^{(i)}(\boldsymbol{\xi}^{(i)}) + \sum_{\lambda=1}^3 \sum_{\mu=\lambda}^3 A_{\lambda\mu}^{(i)}(\mathbf{x}, t) H_{\lambda\mu}^{(2)}(\boldsymbol{\xi}^{(i)}) + \dots \right\} \quad (8)$$

In this paper, the order of the Hermite expansion is taken up to 2. For our problem, the initial conditions are

$$\mathbf{v} = v_0^{(i)} \mathbf{e}_1, \quad p_0^{(i)} = k_B n_0 T_0, \quad v_0^{(i)}, p_0^{(i)}, n_0^{(i)}, T_0^{(i)} = \text{const.}$$

Therefore, the initial conditions imply that physical variables depend only time, and are spatial uniformity. These give

$$A_1^{(i)} = 1, \quad A_2^{(i)} = A_3^{(i)} = A_{12}^{(i)} = A_{13}^{(i)} = A_{23}^{(i)} = 0, \quad A_{22}^{(i)} = A_{33}^{(i)}. \quad (9)$$

Thus, we have six variables  $A_1^{(i)}, A_{11}^{(i)}, A_{22}^{(i)}$  ( $i=1,2$ ).

## DERIVATION OF THE DIFFERENTIAL EQUATIONS FOR THE HERMITE EXPANSION COEFFICIENTS

The Galerkin method is applied:

$$\left. \begin{aligned} \iiint H_0^{(0)}(\boldsymbol{\xi}^{(i)}) B(f^{(i)}, f^{(j)}) d^3 \boldsymbol{\xi}^{(i)} &= 0 \\ \iiint H_1^{(1)}(\boldsymbol{\xi}^{(i)}) B(f^{(i)}, f^{(j)}) d^3 \boldsymbol{\xi}^{(i)} &= 0 \\ \iiint H_{11}^{(2)}(\boldsymbol{\xi}^{(i)}) B(f^{(i)}, f^{(j)}) d^3 \boldsymbol{\xi}^{(i)} &= 0 \\ \iiint H_{22}^{(2)}(\boldsymbol{\xi}^{(i)}) B(f^{(i)}, f^{(j)}) d^3 \boldsymbol{\xi}^{(i)} &= 0 \end{aligned} \right\} \quad (10)$$

From these equations, the differential equations for  $A_1^{(i)}, A_{11}^{(i)}, A_{22}^{(i)}$  are obtained. The system of differential equations could be described with a matrix form as follows,

$$\begin{aligned} & \frac{\partial}{\partial t} \begin{pmatrix} A_0^{(i)} \\ A_1^{(i)} \\ A_{11}^{(i)} \\ A_{22}^{(i)} \end{pmatrix} + \begin{pmatrix} C_{0,0}^{(i)} & 0 & 0 & 0 \\ C_{1,0}^{(i)} & 0 & 0 & 0 \\ C_{11,0}^{(i)} & 0 & C_{11,11}^{(i)} & 0 \\ C_{22,0}^{(i)} & 0 & 0 & C_{22,22}^{(i)} \end{pmatrix} \begin{pmatrix} A_0^{(i)} \\ A_1^{(i)} \\ A_{11}^{(i)} \\ A_{22}^{(i)} \end{pmatrix} \\ & + \mathbf{n}^{(j)} \left\{ A_0^{(j)} \begin{pmatrix} 0 & 0 & 0 & 0 \\ D_{1,0,0}^{(ij)} & 0 & 0 & 0 \\ D_{11,0,0}^{(ij)} & 0 & D_{11,11,0}^{(ij)} & 0 \\ D_{22,0,0}^{(ij)} & 0 & 0 & D_{22,22,0}^{(ij)} \end{pmatrix} \begin{pmatrix} A_0^{(i)} \\ A_1^{(i)} \\ A_{11}^{(i)} \\ A_{22}^{(i)} \end{pmatrix} + A_0^{(i)} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & D_{11,0,11}^{(ij)} & 0 \\ 0 & 0 & 0 & D_{22,0,22}^{(ij)} \end{pmatrix} \begin{pmatrix} A_0^{(j)} \\ A_1^{(j)} \\ A_{11}^{(j)} \\ A_{22}^{(j)} \end{pmatrix} \right\} = 0, \quad (11) \end{aligned}$$

$C_{0,0}^{(i)} \sim C_{22,22}^{(i)}$  and  $D_{1,0,0}^{(ij)} \sim D_{22,22,0}^{(ij)}$  are expressed by scalar products of the Hermite functions,  $f_M^{(i)}(\boldsymbol{\xi}^{(i)})$  etc. The scalar products are defined:

$$(F(\boldsymbol{\xi}_1^{(i)}), G(\boldsymbol{\xi}^{(j)}))_i = \iiint_{\boldsymbol{\xi}_1^{(i)}} \iint_k F(\boldsymbol{\xi}_1^{(i)}) G(\boldsymbol{\xi}^{(j)}) k_c^{(ij)} d^2 \mathbf{k} d^3 \boldsymbol{\xi}_1^{(i)} \quad (12)$$

## THE DEFINITION OF THE DIFFERENTIAL CROSS SECTION

We define the intermolecular force consisting of an inverse fifth- and third-order power, which are respectively repulsive in inner range and attractive in the outer range, of intermolecular distance. This potential is described as

$$U = -\frac{\kappa_a}{r^4} + \frac{\kappa_b}{r^2} \quad (13)$$

The depth of the intermolecular potential is  $U_0 = -\kappa_b^2 / (4\kappa_a)$  at the position  $\delta = \sqrt{2\kappa_a / \kappa_b}$  where the r-differential of the potential is equal to zero. The distance at this point  $\delta$  from the center of  $i$ -molecule could be considered as the molecular size. Using of this intermolecular potential and the kinetic energy  $E = \mu g^2 / 2$  of  $i$ - and  $j$ -molecules with the effective mass  $\mu$  and the relative velocity  $g = |\mathbf{c}^{(j)} - \mathbf{c}^{(i)}|$ . By taking second order of the elliptic function obtained from the orbital integration,  $k_C^{(ij)}$  is obtained as

$$k_C^{(ij)} = \pi^2 \left( -(\pi^2 - 6) \frac{\kappa_b}{\mu} + 3 \sqrt{9 \left( \frac{2\kappa_b}{\mu} \right)^2 + \frac{\kappa_a}{4\mu} (24 - \pi^2)(\pi^2 + 12) g^2} \right) / \left( (24 - \pi^2)(\pi^2 + 12) g \right). \quad (14)$$

In this paper, as an approximation, the relative velocity  $g$  could be changed to the mean value as,

$$\bar{g} = \sqrt{\frac{1}{n^{(i)} n^{(j)}} \int (\mathbf{c}^{(j)} - \mathbf{c}^{(i)})^2 f^{(i)} f^{(j)} d\mathbf{c}^{(i)} d\mathbf{c}^{(j)}} = \sqrt{3k_B \left( \frac{T^{(i)}}{m^{(i)}} + \frac{T^{(j)}}{m^{(j)}} \right) + (\mathbf{v}^{(j)} - \mathbf{v}^{(i)})^2}, \quad (15)$$

which was proposed by one of authors(S.K.)<sup>2</sup>.

## THE ASYMPTOTIC VALUE OF THE MEAN VELOCITY AND THE TEMPERATURE

The final velocity  $\mathbf{v}_\infty = \mathbf{v}_\infty^{(i)} = \mathbf{v}_\infty^{(j)}$  can be estimated from the conservation of momentum:

$$m^{(1)} n_0^{(1)} \mathbf{v}_0^{(1)} + m^{(2)} n_0^{(2)} \mathbf{v}_0^{(2)} = (m^{(1)} n_0^{(1)} + m^{(2)} n_0^{(2)}) \mathbf{v}_\infty$$

From this, we can get

$$\mathbf{v}_\infty = \frac{m^{(1)} n_0^{(1)} \mathbf{v}_0^{(1)} + m^{(2)} n_0^{(2)} \mathbf{v}_0^{(2)}}{m^{(1)} n_0^{(1)} + m^{(2)} n_0^{(2)}} \quad (16)$$

Similarly, the final temperature  $T_\infty = T_\infty^{(i)} = T_\infty^{(j)}$  can be also obtained from conservation of energy:

$$\frac{3}{2} k_B n_0^{(1)} T_0^{(1)} + \frac{3}{2} k_B n_0^{(2)} T_0^{(2)} + \frac{1}{2} m^{(1)} n_0^{(1)} \mathbf{v}_0^{(1)2} + \frac{1}{2} m^{(2)} n_0^{(2)} \mathbf{v}_0^{(2)2} = \frac{3}{2} k_B (n_0^{(1)} + n_0^{(2)}) T_\infty + \frac{1}{2} (m^{(1)} n_0^{(1)} + m^{(2)} n_0^{(2)}) \mathbf{v}_\infty^2$$

From this, we can get

$$T_\infty = \frac{n^{(1)} T_0^{(1)} + n^{(2)} T_0^{(2)}}{n^{(1)} + n^{(2)}} + \frac{n^{(1)} n^{(2)} m^{(1)} m^{(2)} (\mathbf{v}_0^{(1)} - \mathbf{v}_0^{(2)})^2}{3k_B (n^{(1)} + n^{(2)}) (n^{(1)} m^{(1)} + n^{(2)} m^{(2)})} \quad (17)$$

## NUMERICAL RESULTS

In the calculation of the equation obtained above, the molecular diameter  $\delta^{(12)}$ , the collision time  $\tau_c^{(2)}$  and the thermal velocity  $c_m^{(2)}$  of the second gas are chosen with superscript as unit of non-dimensionalization of them:

$$\frac{t}{\tau_c^{(2)}} \rightarrow t^*, \quad \frac{\mathbf{x}}{\delta^{(12)}} \rightarrow \mathbf{x}^*, \quad \frac{\mathbf{v}^{(i)}}{c_m^{(2)}} \rightarrow \mathbf{v}^{(i)*}, \quad \frac{\alpha^{(i-1)}}{c_m^{(2)}} \rightarrow \alpha^{(i)*-1}, \quad \frac{\alpha^{(i-3)}}{n_0^{(2)}} f^{(i)} \rightarrow f^{(i)*}, \quad J^{(ij)} \rightarrow n_0^{(2)} \delta^{(12)3} J^{(ij)*}$$

Because  $\tau_c^{(2)} c_m^{(2)} / \delta^{(12)} = 1$ , the non-dimensional Boltzmann equation, removed \*, is obtained with the coefficient of the collision term such as  $n_0^{(2)} \delta^{(12)^3}$ . It is approximately equal one because of  $\ell_n^3 = 1/n_0^{(2)}$  and  $\delta^{(12)^3} / \ell_n^3 \approx 1$ . In the numerical calculations, the initial are put as (1)  $m^{(1)} = 4, m^{(2)} = 1, T_0^{(1)} = 1.5, T_0^{(2)} = 1, v_0^{(1)} = 0, v_0^{(2)} = 0, \kappa_a = 2, \kappa_b = 4$ , (2)  $m^{(1)} = 4, m^{(2)} = 1, T_0^{(1)} = 1, T_0^{(2)} = 1, v_0^{(1)} = 2, v_0^{(2)} = 0, \kappa_a = 2, \kappa_b = 4$ , (3-1)  $m^{(1)} = 4, m^{(2)} = 1, T_0^{(1)} = 1.5, T_0^{(2)} = 1, v_0^{(1)} = 2, v_0^{(2)} = 0, \kappa_a = 2, \kappa_b = 4$ , (3-2)  $m^{(1)} = 60, m^{(2)} = 1, T_0^{(1)} = 1.5, T_0^{(2)} = 1, v_0^{(1)} = 2, v_0^{(2)} = 0, \kappa_a = 2, \kappa_b = 4$ , (3-3)  $m^{(1)} = 60, m^{(2)} = 1, T_0^{(1)} = 1.5, T_0^{(2)} = 1, v_0^{(1)} = 2, v_0^{(2)} = 0, \kappa_a = 2, \kappa_b = 40$ . The numerical calculations give that the relaxation time for velocity and temperature are the same order for mass ratio of the order one but the relaxation time of temperatures is much longer than that of velocity for much different masses. The calculated values of final velocity and final temperature are almost equal to these obtained from the conservation laws.

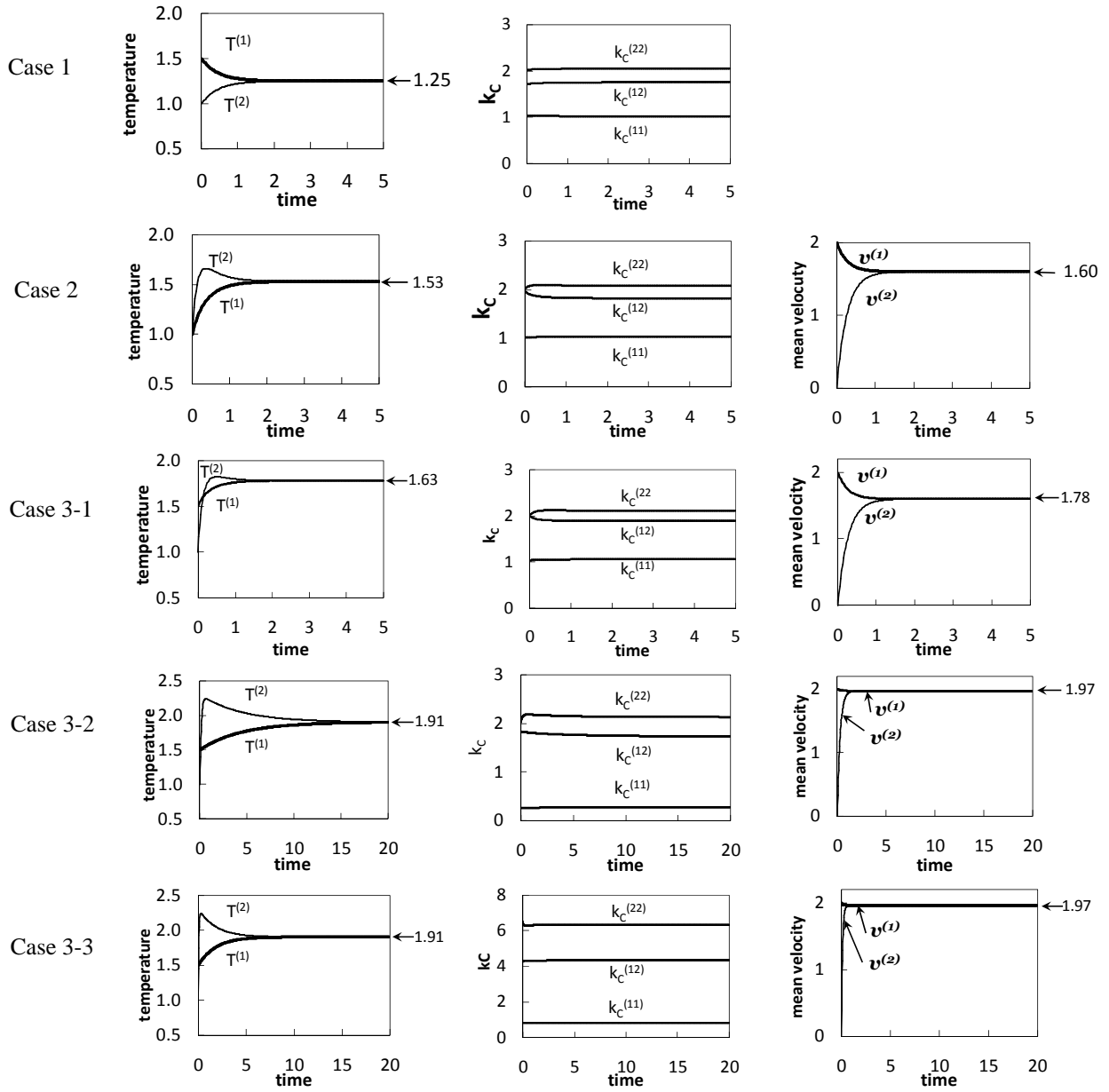


FIGURE 1. The calculation results are shown for five cases.

## **SUMMERY**

The relaxation phenomena of binary gas-mixture with different velocities and different temperatures are discussed on the basis of two Boltzmann equations. The distribution functions of both gases are expanded by Hermite functions of H.Grad. Applying the Garelkin method to solve the Boltzmann equations, we have a system of differential equations of the expansion coefficients. From the conservation of momentum and energy, we can get final values of velocity and temperatures by use of initial ones. The numerical conditions are done for five cases varying initial conditions of velocity and temperature and of different mass ratios. The numerical asymptotic values of velocity and temperature are equal to those obtained by conservation laws. The results of numerical calculations show also that for the cases with the mass ratio of the order one the relaxation times of temperature and velocity are of the same order and the relaxation time for temperature is much longer than that of velocity for the cases for much different masses.

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