

TEMPERATURE DEVELOPMENT IN A PARTIALLY  
IONIZED, REACTING GAS UNDER UNSTEADY  
IONIZATION CONDITIONS

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A solution is presented for the thermal and ionization balance equations for a partially ionized, binary, reacting, multicomponent gas mixture. The conditions for establishment of the temperature of the gas mixture components and of the electron concentration under unsteady ionization conditions are analyzed as a function of the secondary electron energy.

The thermal regime for nonequilibrium ionization conditions in a partially ionized gas mixture with defined chemical kinetics is studied. The limit on ionization ( $x = n_e/n \leq 10^6$ , where  $n_e$  and  $n$  are the electron and neutral concentrations, respectively) assumed in the work ensures that the neutral component properties are thermally static. This limit allows the basic equations to be simplified substantially.

The energy conservation and transport equations for a reacting, binary, spatially uniform gas mixture may be represented in the form [1]

$$3kn_x \frac{dT_x}{dt} = \sum_{\gamma} \eta_{x\gamma} n_x n_{\gamma} (m_x T_x + m_{\gamma} T_{\gamma})^{1/2} (T_{\gamma} - T_x) - \sum_{\gamma'} \beta_{x\gamma'} \frac{T_x^2 n_x n_{\gamma'}}{(m_x T_{\gamma'} + m_{\gamma'} T_x)^{1/2}} + \sum_{\alpha, \beta} \beta_{\alpha\beta} \frac{C^{\alpha\beta} T_x T_{\beta} n_{\alpha} n_{\beta}}{(m_{\alpha} T_{\beta} + m_{\beta} T_{\alpha})^{1/2}} \quad (1)$$

$$\frac{dn_x}{dt} = q_x - \sum_{\gamma'} \alpha_{x\gamma'} n_{\gamma'} n_x + \sum_{\alpha, \beta} \alpha_{\alpha\beta} n_{\alpha} n_{\beta} \quad (2)$$

where

$$C^{\alpha\beta} = 1 + \frac{4m_{\alpha} T_{\beta}}{3m_{\beta} T_{\alpha}} - \frac{4(2m_{\alpha} + m_{\beta})(m_{\alpha} T_{\beta} + m_{\beta} T_{\alpha})}{3m_{\beta} T_{\alpha} (m_{\alpha} + m_{\beta})} + \frac{4(m_{\alpha} m_x + m_x m_{\lambda} + m_{\beta} m_{\lambda})(m_{\alpha} T_{\beta} + m_{\beta} T_{\alpha})^2}{3m_{\beta} m_x (m_{\alpha} + m_{\beta})^2 T_{\alpha} T_{\beta}} + \frac{2\varepsilon_0^{\alpha\beta} m_{\lambda} (m_{\alpha} T_{\beta} + m_{\beta} T_{\alpha})}{3m_x (m_{\alpha} + m_{\beta}) k T_{\alpha} T_{\beta}} - \frac{T_x (m_{\alpha} T_{\beta} + m_{\beta} T_{\alpha})}{m_x T_{\alpha} T_{\beta}}$$

Here  $n_{\kappa}$ ,  $T_{\kappa}$ , and  $m_{\kappa}$  are the concentration, temperature, and mass of particles of the  $\kappa$  component;  $k$  is Boltzmann's constant;  $q_{\kappa}$  is the rate of formation of  $\kappa$ -type particles as the result of external processes; and  $\alpha_{\kappa\gamma}$ ,  $\alpha_{\alpha\beta}$  are the rate constants for creation and annihilation of  $\kappa$ -type particles.

The first term on the right side of Eq. (1) relates to elastic interactions of the  $\kappa$ -th and  $\gamma$ -th components of the mixture, the second sum corresponds to reactions of the form  $\kappa + \gamma' \rightarrow \alpha + \beta$ , and the third sum to reactions of the form  $\alpha + \beta \rightarrow \kappa + \lambda$  (correspondingly,  $\varepsilon_0^{\alpha\beta}$  is the energy effect of this reaction).

The coefficients under the summation sign on the right side of Eq. (1) are determined by the interaction cross section

$$\eta_{x\gamma} = \frac{32 \sqrt{\pi} \sigma_{x\gamma} k^{3/2} (m_x m_{\gamma})^{1/2}}{\sqrt{2} (m_x + m_{\gamma})^2} \quad (3)$$

$$\beta_{x\gamma'} = \frac{4 \sqrt{2\pi} \sigma_{x\gamma'}^* k^{3/2} m_{\gamma'}^{1/2}}{m_x^{1/2}}, \quad \beta_{\alpha\beta} = \frac{12 \sqrt{2\pi} \sigma_{\alpha\beta}^* k^{3/2} m_x}{(m_{\alpha} m_{\beta})^{1/2}} \quad (4)$$

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Here  $\sigma_{\chi\gamma}$  is the differential cross section for elastic interactions and  $\sigma_{\chi\gamma}^*$ ,  $\sigma_{\alpha\beta}^*$  are the differential cross sections for inelastic interactions.

The set of Eqs. (1) and (2) is nonlinear and the possibility of its linearization is associated with limiting the degree of ionization. This permits consideration of only neutral components in the gas medium in accounting for elastic collision interactions.

Then, from Eqs. (1) and (2), the equations which determine the electron temperature and concentration take the form

$$kn_e \frac{dT_e}{dt} = \sum_{\gamma} \frac{32 \sqrt{\pi} \sigma_{e\gamma} k^{3/2} (m_e m_{\gamma})^{1/2} n_e n_{\gamma} (m_e T_e + m_{\gamma} T_{\gamma})^{1/2}}{3 \sqrt{2} (m_e + m_{\gamma})^2} \times (T_{\gamma} - T_e) - \frac{4 \sqrt{2\pi} n_e (kT_e)^{1/2}}{3m_e^{3/2}} \sum_i \sigma_{ei} n_i + (\varepsilon_e - 3kT_e) q \quad (5)$$

$$\frac{dn_e}{dt} = q + n_e \sum_i \alpha_{ei} n_i \quad (6)$$

and the ion temperature under quasineutral,  $n_e = \sum n_i$ , and thermally static conditions,  $T_n = \text{const}$  (the index relates to neutral particles), may be found from the equation

$$(T_n - T_i) (T_i + T_n)^{1/2} = (T_e - T_n) T_n^{1/2} \frac{4\sigma_{en} m_e^{3/2}}{\sigma_{in} m_n^{3/2}} \quad (7)$$

For solution of Eq. (7) it is convenient to introduce the notation

$$(T_e - T_n) T_n^{1/2} \frac{4\sigma_{en} m_e^{3/2}}{\sigma_{in} m_n^{3/2}} = c, \quad \cos \varphi = \frac{1}{2} \left( 2 - \frac{27c^2}{(2T_n)^3} \right)$$

The energy relationship for the reacting system has the form

$$M_i + h\nu_l = M_i^+ + e$$

where  $l = 1, 2, \dots, k$  corresponds to the characteristic ionizing radiation frequency, determined by the electron concentration of the gas mixture without account of additional heat sources, and is characterized by two fundamental values: the ionization rate  $q = q_1 + q_2 + \dots + q_k$ ; and the mean energy effect of the reaction, i.e., the average secondary electron energy

$$\varepsilon_e = \frac{n_1 \varepsilon_1 + n_2 \varepsilon_2 + \dots + n_k \varepsilon_k}{n_1 + n_2 + \dots + n_k} \quad (8)$$

It is known that the relationship between these values is one of the most significant characteristics of heat transfer. Thus, establishing this relationship together with determination of the temperature development time is the primary aim of this work.

We introduce the average effective values of  $\langle \alpha \rangle$  and  $\langle \sigma^* \rangle$  by the equations†

$$\langle \alpha \rangle = \frac{\sum \alpha_{e\beta} n_{\beta}}{\sum n_{\beta}}, \quad \langle \sigma^* \rangle = \frac{\sum \sigma_{e\gamma}^* n_{\gamma}}{\sum n_{\gamma}}$$

and transform Eqs. (5)-(7) to the form

$$kn_e \frac{dT_e}{dt} = \sum_{\gamma} \frac{32 \sqrt{\pi} \sigma_{e\gamma} k^{3/2} (m_e m_{\gamma})^{1/2} n_e n_{\gamma} (m_e T_e + m_{\gamma} T_{\gamma})^{1/2}}{3 \sqrt{2} (m_e + m_{\gamma})^2} (T_{\gamma} - T_e) - \frac{4 \sqrt{2\pi} \sigma_e^* n_e^2 (kT_e)^{3/2}}{3m_e^{3/2}} + (\varepsilon_e - 3kT_e) q \quad (9)$$

$$\frac{dn_e}{dt} = q - \alpha n_e^2 \quad (10)$$

$$T_i = T_n \left( \frac{1}{3} + \frac{4}{3} \cos(60^\circ - \frac{1}{3}\varphi) \right) \quad (11)$$

† In the following the  $\langle \rangle$  will be deleted, i.e., it shall be understood that  $\alpha$  and  $\sigma^*$  refer to the average values.

Transforming to the dimensionless variables

$$z = n_e/n, \quad y_e = T_e/T_{0e}, \quad q_e = q/n$$

and taking into account the known relationship between the differential cross sections of the dissociation-recombination reaction and the effective recombination coefficient

$$\sigma^* = \frac{\alpha m_e^{1/2}}{4 \sqrt{2\pi} k T_e^{1/2}}$$

we transform Eq. (9) to the following form:

$$\begin{aligned} \frac{dy_e}{dt} &= - \left( a + \frac{3q_e}{z} + bz \right) y_e + \left( ay + \frac{\varepsilon_e q_e}{k T_{0e} z} \right) \\ a &= \sum_{\gamma} \frac{32 \sqrt{\pi} m_e^{1/2} \sigma_{e\gamma} (k T_n)^{1/2} n_{\gamma}}{3 \sqrt{2} m_{\gamma}}, \quad b = \frac{n\alpha}{3}, \quad y = \frac{T_n}{T_{0e}} \end{aligned} \quad (12)$$

Here  $T_{0e}$  is the initial electron temperature.

In this case, solution of Eq. (12) may be obtained in the following manner:

$$y_e = \exp \left( - \int_0^t \left( a + \frac{3q_e}{z} + bz \right) d\tau \right) \left[ 1 + \int_0^t \left( ay + \frac{\varepsilon_e q_e}{k T_{0e} z} \right) \exp \left( \int_0^{\tau} \left( a + \frac{3q_e}{z} + bz \right) d\gamma \right) d\tau \right] \quad (13)$$

The most general case in which it is convenient to use experimental data in the analysis is the case of rapid change in ionization rate when the function  $q(t)$  may be approximated by the step function

$$q(t) = q_0 + \theta(t) \Delta q, \quad \theta(t) = \begin{cases} 1 & (t \geq 0) \\ 0 & (t < 0) \end{cases}$$

We represent solution of Eq. (10) in the form

$$z = \frac{1}{n} \left( \sqrt{\frac{q_0}{\alpha}} \right)^{1/2} \frac{1 + \omega \operatorname{th}(t \sqrt{\alpha q})}{1 + \omega^{-1} \operatorname{th}(t \sqrt{\alpha q})}, \quad \omega = \left( \frac{q}{q_0} \right)^{1/2} \quad (14)$$

Putting Eq. (14) into (13) we obtain

$$\begin{aligned} y_e &= \left[ \left\{ \frac{u^r - 1}{2r} \left( \frac{\varepsilon_e}{k T_{0e}} - \frac{ay}{\sqrt{\alpha q}} \right) + \frac{u^{r+1} - 1}{2(r+1)} \gamma \left( \frac{3ay}{\sqrt{\alpha q}} - \frac{\varepsilon_e}{k T_{0e}} \right) \right. \right. \\ &\left. \left. - \frac{u^{r+2} - 1}{2(r+2)} \gamma^2 \left( \frac{3ay}{\sqrt{\alpha q}} + \frac{\varepsilon_e}{k T_{0e}} \right) + \frac{u^{r+3} - 1}{2(r+3)} \gamma^3 \left( \frac{ay}{\sqrt{\alpha q}} + \frac{\varepsilon_e}{k T_{0e}} \right) \right\} \gamma^{b/n\alpha} + (\gamma - 1)^3 (\gamma + 1)^{b/n\alpha} \right] u^{-(r+3)} (\gamma - u^{-1})^{-3} (\gamma + u^{-1})^{-b/n\alpha} \end{aligned} \quad (15)$$

where

$$\begin{aligned} u &= \exp(2t \sqrt{\alpha q}), \quad r = \frac{1}{2} \left( \frac{a}{\sqrt{\alpha q}} - 3 + \frac{b}{n\alpha} \right) \\ \gamma &= \begin{cases} (\omega + 1)/(\omega - 1) & \text{for } \omega > 1 \\ -(\omega + 1)/(\omega - 1) & \text{for } \omega < 1 \end{cases} \end{aligned}$$

We determine the rate of development of electron concentration and temperature, i.e., the values which characterize the time rate of approach of  $z$  and  $y_e$  to their asymptotic values.

As a criterion for steady state development we select the conditions

$$|z - z_a| \leq \delta |z_0 - z_a|, \quad |y_e - y_a| \leq \delta_1 |1 - y_a| \quad (16)$$

Here  $\delta$  and  $\delta_1$  are arbitrary positive numbers, and  $y_a$  and  $z_a$  are the asymptotic values of  $y_e$  and  $z$ . Using Eq. (16) we obtain, in analogy with [2], an estimate of the time for establishment of the electron concentration:

$$t_z^0 \geq \frac{1}{2 \sqrt{\alpha q}} \ln \frac{2 - \delta (1 - \omega^{-1})}{\delta (1 + \omega^{-1})} \quad (17)$$

TABLE 1

$q \text{ cm}^{-3} \cdot \text{sec}^{-1}$	$10^5$	$10^4$	$10^3$	$10^2$	
$\varepsilon_{eV} = 0.7$	1.8	5.7	22		$(\lambda = 10)$
$\varepsilon_{eV} = 0.8$	2	5.7	17.5		$(\lambda = 100)$

Equation (17) permits estimation of the time for establishment of the electron temperature  $t_{ye}$ , °K, as a function of  $\delta_1$ . Therefore, if it is assumed that  $t_z$ , °K =  $t_{ye}$ , °K, we obtain the relationship  $\delta_1 = f(\delta)$ . For sufficiently large values of  $t_z$ , °K corresponding to small values of  $\delta$ , it may easily be seen that  $\delta_1 = \delta\lambda$ , while  $z_0 = n_{0e}/n$  ( $n_{0e}$  is the initial value of the electron concentration),

$$\lambda = \frac{z_0 - z_a}{1 - y_a} \lim_{t \rightarrow \infty} \frac{y_e - y_a}{z - z_a} = \frac{[(3 - \vartheta)\eta y - \xi(2\vartheta + \eta)](\omega^{-1} - 1)}{(1 + \vartheta + \eta)[(\eta + 3 + \vartheta) - (\eta y + \xi)]}$$

$$\vartheta = \frac{b}{nx}, \quad \eta = \frac{a}{V\alpha q}, \quad \xi = \frac{\varepsilon_e}{kT_{0e}}$$

Using this fact we obtain the equations for the relationship between  $\varepsilon_e$  and  $q$  knowing, for example,  $\lambda$  from experiment:

$$\varepsilon_e = kT_{0e} \frac{\Psi}{\Phi} \lambda - \frac{\eta k T_n}{\omega \Phi} [\lambda \Psi + (3 - \vartheta)(\omega^{-1} - 1)] \quad (18)$$

$$\Psi = (1 + \vartheta + \eta)(3 + \vartheta + \eta) \quad (19)$$

$$\Phi = \lambda(1 + \vartheta + \eta) - (2\vartheta + \eta)(\omega^{-1} - 1) \quad (20)$$

As an example of the use of the relationships obtained, we estimate the time for establishment of  $n_e$  and  $T_e$  characteristic for the auroral ionosphere, i.e., the region of the ionosphere in which the dominant role in the energy balance and ionization is played by a flow of electrons with a density  $I_e = 10^6 - 10^8 \text{ cm}^{-2} \times \text{sec}^{-1}$  and an energy of 1-10 keV [3]. Computations show that for  $q_0 = 10^3 \text{ cm}^{-3} \text{ sec}^{-1}$

$$n_e = n_i = 10^6 \text{ cm}^{-3}, \quad \alpha = 10^{-7} \text{ cm}^3 \cdot \text{sec}^{-1}$$

$$t_z = \begin{cases} 25 \text{ sec} & \text{for } q = 10^4 \text{ cm}^3 \cdot \text{sec}^{-1} \\ 10 \text{ sec} & \text{for } q = 10^5 \text{ cm}^3 \cdot \text{sec}^{-1} \end{cases}$$

Using the relationship between the secondary electron energy and the change in ionization function, we compute, for values of the parameter  $\lambda = 10$  and  $10^2$ , values of  $T_{0e} = 10^3$  °K and  $T_n = 3 \cdot 10^2$  °K for  $q_0 = 10^3 \text{ cm}^{-3} \text{ sec}^{-1}$ . It may be seen that these values, which are shown in Table 1, are in agreement with one another. Actually, increase in the ionization rate, and correspondingly in the density of heating sources in the gas mixture, leads to much more intense heat transfer (decrease in temperature establishment time) and decrease in the energy of secondary, hyperthermal electrons.

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