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DETERMINATION OF THE SPECIFIC HEAT RELEASE IN POLAR GASES AND FLUIDS IN A VARIABLE ELECTRIC FIELD

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The Debye model of interaction of a polar molecule with an electric field and the medium surrounding the molecule is applied for numerical determination of the specific heat release in gaseous ammonia, steam, and in water attributed to dissipation of the energy of a variable electric field in a viscous polar medium.

Under the action of a variable electric field a gas or a liquid molecule possessing an electric dipole moment performs vibrational–rotational motion in a viscous medium around the axis perpendicular to its dipole moment, which is accompanied by conversion of the kinetic energy of the rotational motion of the molecule into thermal energy [1].

The aim of the present work is to calculate the amount of heat released for unit time per unit volume of the medium by using the equation of motion of a dipole in a variable electric field.

In the calculations we used the Debye molecule in which a molecule was considered as a sphere possessing the dipole moment of an actual molecule, while the molecules surrounding it were assumed to be a viscous continuum described by the equations of hydrodynamics [1].

The calculations were carried out for a field with a circular frequency of $\omega = 1.54 \cdot 10^{10}$ rad/sec. At such a frequency the electronic and vibrational states of molecules are virtually not excited [2].

A polar molecule in an electric field is subjected to the action of a moment of force $k = -\partial u / \partial \vartheta$, where u is the scalar product of the electric-field intensity **E** by a dipole moment **d**, taken with an inverse sign, i.e., $u = -\sum_i d_i E_i$, and ϑ is the angle formed by **E** and **d**.

We assume that the field is directed along the polar z-axis; this gives $u = -d_z E_z$.

Let us consider the simplest case where $E_z = E_0 \cos \omega t$.

The product of the moment of inertia of the molecule I by the angular acceleration $\ddot{\vartheta}$ is equal to the sum of the moments of forces acting on the dipole [3].

To the dipole the moment of the force attributable to an electric field i.e., $k = -dE \sin \vartheta$, and the moment of the viscous force proportional to the angular rotational velocity of the molecule ϑ are applied.

An analytical expression for the moment of the viscous force is known only in the simplest case of a rotating sphere [1] and is written as

$$M = -\xi \dot{\vartheta} ,$$

where $\xi = 8\pi\eta R^3$; here R is the sphere radius.

With regard for the foregoing, the equation of motion of an electric dipole in the field of an electromagnetic wave can be represented in the form

$$I\ddot{\vartheta} = -dE_0 \cos \omega t \sin \vartheta - \xi \dot{\vartheta} . \qquad (1)$$

After multiplying (1) by $\dot{\vartheta}$ with account for $\dot{\vartheta}\ddot{\vartheta} = \frac{d}{dt}\left(\frac{\dot{\vartheta}^2}{2}\right)$ the expression for the time derivative of the kinetic energy is written as

$$\frac{d}{dt}\left(\frac{I\dot{\vartheta}^2}{2}\right) = dE_0 \cos \omega t \, \frac{d(\cos \vartheta)}{dt} - \xi \dot{\vartheta}^2 . \qquad (2)$$

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It is known that the time derivative of the kinetic energy is equal to the sum of powers of the forces acting on a body [3].

The first term on the right-hand side of Eq. (2) determines the work per unit time done by an electric field on a dipole, while the second term is the work per unit time done by the viscous force on the dipole. The first term determines the kinetic energy of the molecule and can be both positive and negative, while the second term is always negative. Precisely the second term is responsible for dissipation of the kinetic energy into the thermal one.

We assume that at a certain instant of time an electric field can be switched off; then Eq. (2) can be represented as follows

$$\frac{d}{dt}\left(\frac{I\dot{\vartheta}^2}{2}\right) = -\xi\,\dot{\vartheta}^2 . \tag{3}$$

A solution of Eq. (3) is written in the form

$$\dot{\vartheta}^2 = \dot{\vartheta}_0^2 \exp\left(-\frac{2\xi}{I}t\right) = \dot{\vartheta}_0^2 \exp\left(-\frac{t}{\tau}\right), \tag{4}$$

where $\tau = I/2\xi = I/(16\pi\eta R^3)$ is the time of viscous relaxation for which the kinetic energy of the rotational motion of a molecule decreases e times.

We will evaluate this time for the molecule of gaseous ammonia. In this case, $R \approx 2\cdot 10^{-10}$ m, $M = 2.9\cdot 10^{-26}$ kg, $I = \frac{2}{5}MR^2 \approx 5\cdot 10^{-46}$ kg·m^2, and $\eta \approx 10^{-5}$ kg/(m·sec), whence $\tau \approx 10^{-13}$ sec.

Next, Eq. (1) can be represented as

$$\ddot{\vartheta} + \omega_1\dot{\vartheta} + \omega_0^2\cos\omega t\sin\vartheta = 0 . \tag{5}$$

Here $\omega_1 = 1/2\pi$ and $\omega_0^2 = dE_0/I$.

To simplify the analysis, it is convenient to write Eq. (5) in dimensionless form. Let us introduce the dimensionless time

$$t' = \frac{t}{T_0} = \frac{\omega_0}{2\pi}t, \quad \text{then} \quad \frac{d\dot{\vartheta}}{dt} = \frac{\omega_0}{2\pi}\frac{d\vartheta}{dt}, \ \frac{d^2\vartheta}{dt^2} = \left(\frac{\omega_0}{2\pi}\right)^2\frac{d^2\vartheta}{dt'^2}, \ \cos\omega t = \cos\left(2\pi\frac{\omega}{\omega_0}t'\right).$$

As a result, Eq. (5) acquires the form

$$\frac{d^2\vartheta}{dt^2} + 2\pi\frac{\omega_1}{\omega_0}\frac{d\vartheta}{dt} + (2\pi)^2\cos\left(2\pi\frac{\omega}{\omega_0}t\right)\sin\vartheta = 0 . \tag{6}$$

Hereafter the prime in the dimensionless time is omitted.

Solution of Eq. (1) depends on two dimensionless parameters, i.e., $\alpha = \omega_1/\omega_0$ and $\beta = \omega/\omega_0$.

In Table 1 the values of α and β are given for the gaseous ammonia at room temperature and normal pressure, for steam at room temperature and a pressure of $2.6\cdot 10^3$ Pa, and for water at the same temperature at different values of the field amplitude E_0. The values of α change from hundreds to hundreds of thousands, and the values of β are in the interval between one and ten.

We will evaluate the first and second terms of Eq. (6) with respect to the order of magnitude. Provided the dimensional time is equal to the period of an electric field T, the dimensionless time is equal to ω_0/ω. With regard for this, the derivative $d\vartheta/dt$ becomes, with respect to the order of magnitude, $\beta = \omega_0/\omega$, while the second derivative becomes $\beta^2 = (\omega/\omega_0)^2$.

The ratio of the first term of the equation to the second term appears to be $\beta/(2\pi\alpha) << 1$. This indicates that the nonlinear differential equation of second order degenerates into the equation of first order [4]

$$\frac{d\vartheta}{dt} + \frac{2\pi}{\alpha} \cos (2\pi\beta t) \sin \vartheta = 0 \, . \tag{7}$$

Below we give the results for the specific heat release obtained from an analytical solution of the degenerate equation of first order (7) and from a numerical solution of the initial equation of second order (6).

An analytical solution of (7) in the implicit form is written as follows:

$$\tan \frac{\vartheta}{2} = \tan \frac{\vartheta_0}{2} \exp \left(- \frac{1}{\alpha\beta} \sin (2\pi\beta t) \right), \tag{8}$$

where ϑ_0 is the initial value of a polar angle. To determine the heat released, it is necessary to know $\dot{\vartheta}^2$. Simple calculations yield the expression

$$\dot{\vartheta}^2 = \frac{16\pi^2}{\alpha^2} \tan^2 \frac{\vartheta_0}{2} \frac{\exp \left(- \dfrac{2 \sin (2\pi\beta t)}{\alpha\beta} \right) \cos^2 (2\pi\beta t)}{\left(1 + \tan^2 \dfrac{\vartheta_0}{2} \exp \left(- \dfrac{2 \sin (2\pi\beta t)}{\alpha\beta} \right) \right)^2} \, . \tag{9}$$

This expression should be averaged over the initial angles ϑ_0 using the distribution $\sin \vartheta_0 d\vartheta_0 / 2$, $0 \le \vartheta_0 \le \pi$. Here, the symmetry of (9) relative to the polar axis is taken into account. As a result, we arrive at

$$\overline{\dot{\vartheta}^2} = \frac{AQ}{2} \left(\frac{1}{2 (1 + A)} - \frac{1}{(1 - A)^3} \left(2 - 2 (A + 1) \ln 2 - \frac{(1 + A)^2}{2} + 2 (A + 1) \ln (A + 1) \right) \right). \tag{10}$$

Here

$$A = \exp \left(- \frac{2 \sin (2\pi\beta t)}{\alpha\beta} \right), \quad Q = \frac{16\pi^2}{\alpha^2} \cos^2 (2\pi\beta t) \, .$$

Expression (10) should be averaged over the dimensionless time within the limits from 0 to ω_0 / ω, which indicates averaging over the dimensional time for the period of an acting electric field.

Taking into account that $\left| \dfrac{2 \sin (2\pi\beta t)}{\alpha\beta} \right| << 1$, we obtain the expansion of expression (10) with an accuracy of up to $x^2 = \left(\dfrac{2 \sin (2\pi\beta t)}{\alpha\beta} \right)^2$.

Averaging of (11) over the time yields

$$\overline{\dot{\vartheta}^2} \approx \frac{Q}{12} \left(1 + \frac{3}{8} x - \frac{23}{80} x^2 \right). \tag{11}$$

$$\overline{\overline{\dot{\vartheta}}}^{\,2} = \frac{2}{3} \frac{\pi^2}{\alpha^2} \left(1 - \frac{23}{20} \alpha^{-2} \beta^{-2} \right). \tag{12}$$

In the dimensional form, the dissipative function $\dot{E}_\eta$ determining the energy dissipated into heat by one dipole per unit time is written as

$$\dot{E}_\eta = I \left(\frac{\omega_0}{2\pi} \right)^3 \frac{2\pi\omega_1}{\omega_0} \overline{\overline{\dot{\vartheta}}}^{\,2} \, . \tag{13}$$

TABLE 1. Values of the Parameters $\alpha = \omega_1 / \omega_0$ and $\beta = \omega / \omega_0$

Parameters	$E_0 \cdot 10^{-2}$, V/m										
	5	10	15	20	25	40	50	70	90	100	300
	Ammonia										
α	2278	1611	1315	1139	1019	805	720	609	532	509	294
β	7.33	5.19	3.67	3.28	2.59	2.32	1.96	1.73	1.64	0.95	0.78
	Steam										
α	3305	2337	1908	1652	1478	1169	1045	883	779	739	427
β	6.08	4.30	3.50	3.04	2.72	2.15	1.92	1.60	1.40	1.36	0.78
	Water										
α	$1.6 \cdot 10^5$	$1.2 \cdot 10^5$	$9.5 \cdot 10^4$	$8.3 \cdot 10^4$	$7.4 \cdot 10^4$	$5.8 \cdot 10^4$	$5.2 \cdot 10^4$	$4.4 \cdot 10^4$	$3.9 \cdot 10^4$	$3.7 \cdot 10^4$	$2.1 \cdot 10^4$
β	6.1	4.3	3.51	3.04	2.72	2.15	1.92	1.60	1.43	1.36	0.78

Finally

$$\dot{E}_\eta = \frac{1}{6} \dot{I} \omega^3 \frac{1}{\beta^3} \frac{1}{\alpha} \left(1 - \frac{23}{20} \alpha^{-2} \beta^{-2} \right). \tag{14}$$

As follows from the foregoing, expression (14) is valid provided that

$$\frac{\omega_0}{\alpha} << \omega << \pi \omega_1 . \tag{15}$$

In this frequency range of an acting electric field the heat release increases with the frequency.

To obtain the energy loss per unit volume per unit time expression (14) should be multiplied by the number of molecules per unit volume.

It is known that a differential equation of *n*th order is equivalent to a system of *n* differential equations of first order with two unknowns ϑ and $\dot{\vartheta}$. For this we assume that

$$\dot{\vartheta} = \frac{d\vartheta}{dt} , \quad \frac{d\dot{\vartheta}}{dt} = - 2\pi \frac{\omega_1}{\omega_0} \dot{\vartheta} - (2\pi)^2 \cos \left(2\pi \frac{\omega}{\omega_0} t \right) \sin \vartheta . \tag{16}$$

The system of equations (16) was solved numerically by the Euler–Cromer method that had proved itself well in solving equations describing vibrational phenomena [6]. In our case, the Euler–Cromer algorithm acquires the form

$$\vartheta_{n+1} = \vartheta_n + \dot{\vartheta}_{n+1} \Delta t , \quad \dot{\vartheta}_{n+1} = \frac{\dot{\vartheta}_n}{1 + 2\pi \frac{\omega}{\omega_0} \Delta t} - \left((2\pi)^2 \cos \left(2\pi \frac{\omega}{\omega_0} t \right) \sin \vartheta_n \right) \frac{\Delta t}{1 + 2\pi \frac{\omega}{\omega_0} \Delta t} . \tag{17}$$

The system of equations (17) was solved numerically for several values of the initial angle ϑ_0, then a dissipative function for the initial angles $\left(2\pi \frac{\omega_1}{\omega_0} \dot{\vartheta}^2 \right)$ was determined, and next the dissipative function was averaged over the time and the initial angles with allowance for the symmetry relative to the polar axis using the distribution $\sin \vartheta_0 d\vartheta_0 / 2$.

At the values of α and β given in Table 1, a numerical solution of equations (16) is virtually independent of the initial angular velocity $\dot{\vartheta}_0$ and is determined only by the value of the polar angle ϑ_0 at the initial instant of time, which numerically confirms the degeneracy of the equation of second order (6) into the equation of first order (7).

TABLE 2. Calculated Results of Heat Release $\dot{E}_\eta$, $\dot{E}_{\eta\mathrm{m}}$, $\dot{E}_{\eta\mathrm{m\cdot anal}}$ ($\cdot10^6$, W/m^3)

$E_0\cdot10^{-2}$, V/m	$\dot{E}_\eta$ at ϑ_0, deg					$\dot{E}_{\eta\mathrm{m}}$	$\dot{E}_{\eta\mathrm{m\cdot anal}}$
	10	20	50	70	90		
Ammonia							
5	$9\cdot10^{-4}$	$3.6\cdot10^{-3}$	$1.8\cdot10^{-2}$	$2.7\cdot10^{-2}$	$3\cdot10^{-2}$	0.01	0.01
10	$3.7\cdot10^{-3}$	$1.4\cdot10^{-2}$	$7.2\cdot10^{-2}$	0.1	0.12	0.04	0.04
20	$1.5\cdot10^{-2}$	$5.7\cdot10^{-2}$	0.3	0.43	0.49	0.165	0.224
50	$9\cdot10^{-2}$	0.36	1.8	2.7	3.07	1.024	1.6
90	0.3	1.2	5.8	8.75	9.9	3.305	3.92
Steam							
5	$2.5\cdot10^{-6}$	$9.8\cdot10^{-6}$	$5\cdot10^{-5}$	$7.4\cdot10^{-5}$	$8.4\cdot10^{-5}$	$2.8\cdot10^{-5}$	$3\cdot10^{-5}$
10	$1\cdot10^{-5}$	$4\cdot10^{-5}$	$2\cdot10^{-4}$	$3\cdot10^{-4}$	$3.36\cdot10^{-4}$	$1.12\cdot10^{-4}$	$1.13\cdot10^{-4}$
20	$4\cdot10^{-5}$	$1.6\cdot10^{-4}$	$8\cdot10^{-4}$	$1.2\cdot10^{-3}$	$1.34\cdot10^{-3}$	$4.45\cdot10^{-4}$	$4.7\cdot10^{-4}$
50	$2.5\cdot10^{-4}$	$9.8\cdot10^{-4}$	$5\cdot10^{-3}$	$7.4\cdot10^{-3}$	$8.4\cdot10^{-3}$	$2.8\cdot10^{-3}$	$2.82\cdot10^{-3}$
90	$8\cdot10^{-4}$	$3\cdot10^{-3}$	$1.6\cdot10^{-2}$	$2.4\cdot10^{-2}$	$2.7\cdot10^{-2}$	$9\cdot10^{-3}$	$9\cdot10^{-3}$
Water							
5	$2.4\cdot10^{-2}$	$9\cdot10^{-2}$	0.46	0.7	0.79	0.265	0.268
10	$9.5\cdot10^{-2}$	0.37	1.8	2.8	3.16	1.05	1
20	0.38	1.47	7.39	11.12	12.59	4.2	4.35
50	2.38	9.23	46.3	69.65	78.87	26.29	26.5
90	7.66	29.73	149	224	254	84.7	85

Table 2 gives the time-averaged values of heat release $\dot{E}_\eta$ as a function of the initial angle ϑ_0 and of the amplitude of an electric field and the initial angle-averaged values of heat release $\dot{E}_{\eta\mathrm{m}}$ for gaseous ammonia, steam, and water in units of 10^6 W/m^3, obtained on solving numerically the system (16). The same table gives the values of specific heat release (W/m^3) $\dot{E}_{\eta\mathrm{m.anal}}$ calculated with the use of the analytical solution of Eq. (7). The values of $\dot{E}_{\eta\mathrm{m}}$ and $\dot{E}_{\eta\mathrm{m.anal}}$ virtually coincide.

The calculated results have been experimentally tested for two polar media, i.e., distilled water and gaseous ammonia. An experiment was carried out under normal conditions (at atmospheric pressure and an ambient temperature equal to 293 K). The intensity of the electric component of the electromagnetic field was $E_0 \approx 7\cdot10^2$ V/m, and the frequency $\omega = 1.54\cdot10^{10}$ rad/sec. Water and ammonia were placed into a vessel made of radiotransparent material having low conductivity (polytetrafluoroethylene).

We determined the rate of change in the temperature of the medium in the field of an electromagnetic wave. In conformity with this, the specific heat release for distilled water was 10^6 W/m^3, and for ammonia $1.7\cdot10^4$ W/m^3.

The values of the heat release in the indicated media calculated by the suggested method at the same parameters of the electromagnetic field amounted to 10^6 W/m^3 for water and $5\cdot10^4$ W/m^3 for gaseous ammonia. As is seen, the values of the heat release obtained from measurements and those calculated by the suggested method coincide within the limits of the order of magnitude.

Thus, in the present work a procedure is suggested for calculation of the energy losses of an electromagnetic field in polar media. The procedure is based on the Debye model describing interaction of polar molecules with an external variable electric field and a surrounding medium. The calculation is carried out with the use of the prescribed values of the parameters of the electromagnetic field and the reference parameters of the medium.

NOTATION

ω, circular velocity, rad/sec; d, dipole moment, C·m; E_0, amplitude of the electric-field intensity, V/m; I, moment of inertia of the molecule, kg·m^2; M, moment of the viscous force, N·m; η, dynamic viscosity, N·sec/m^2.

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