

Power Dissipation of Uniaxial Anisotropic/Interacting Polar Molecules with Linear Reaction Dynamics in an Alternating Electric Field

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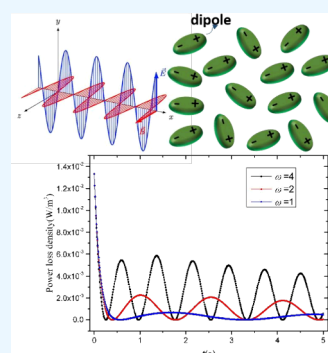
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ABSTRACT: The influence of anisotropic potential energy and interaction between polar molecules on power absorption in chemical reactions with linear reaction dynamics in a weak alternating electric field is studied theoretically according to the reaction-diffusion equation. The expression for transient power loss is derived using two methods, electrodynamic method and equivalent circuit method, based on the electric energy conservation equation. Numerical calculations are carried out, and the results show that both the anisotropic potential energy and the interaction between polar molecules have a strong impact on energy dissipation and storage. For the anisotropic potential energy, when the applied dimensionless anisotropy is equal to 1, the power loss density increases about 32% at a low reaction rate and 27% at a high reaction rate compared to the case without anisotropic potential energy. When the dimensionless anisotropy is equal to -1 , the power loss is suppressed and is reduced about 27% and 24% at low and high reaction rates, respectively. On the other hand, for the interaction between polar molecules, the power loss density decreases about 10% and 30% with low and high interaction potential energies, respectively. In addition, if the reaction rate is relatively high, the power loss will quickly decrease due to the end of the reaction process.



1. INTRODUCTION

Carbon neutrality arouses global attention, which is an inevitable requirement to promote the sustainable and high-quality development of mankind. Improving energy efficiency is one of the effective ways to achieve this goal. Microwave energy is known as an efficient and clean energy, which can significantly improve energy utilization in certain application scenarios, such as application of microwave-assisted hydrothermal extraction in food,^{1,2} microwave drying of food,³ organic/inorganic synthesis,^{4–9} ore refining,^{10–15} and so on. Although microwave energy has the characteristics of high efficiency and rapid heating, the nonuniform heating and thermal runaway limit the large-scale application in industry. In particular, for the microwave heating process of chemical reactions, it is important to understand the energy dissipation mechanism of the chemical reaction system in the presence of electromagnetic fields in order to enhance its safe application. However, relevant basic research is restricted, since the chemical process is dynamic.

For a linear dielectric medium, Debye originally described the dielectric relaxation based on the Smoluchowski-Debye equation,¹⁶ which provides a possibility for research in this field. Then, the dissipation power of microwaves in matter can be described by using the concept of permittivity¹⁷

$$P_{\text{loss}} = \frac{1}{2} \omega \epsilon'' |\vec{E}(\omega)|^2 \quad (1)$$

where \vec{E} , ω , and ϵ'' are the electric field, the angular frequency and the imaginary part of the complex permittivity, respectively. However, it is difficult to characterize the power dissipation of chemical reaction systems in the presence of electromagnetic fields because chemical reactions are a dynamic process accompanied by the generation and consumption of new and old substances. Previous research work has shown that chemical reaction processes may have an impact on the polarization. According to the revised Smoluchowski equation, an analytical expression for polarization in polar molecular reactions was obtained, which laid a theoretical foundation for studying power dissipation.¹⁸ The relationship between chemical reaction time and relaxation time was studied using a continuous time random walk model, when the chemical reaction time is much longer than the relaxation time, the effective dielectric constant can be used to describe the dielectric properties in these reactions.¹⁹ The theory of biased continuous time random walk can more reasonably describe the anomalous dielectric relaxation characteristics of reactions in spatially and temporally depend-

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ent electric fields.²⁰ The same analysis method can also be used in magnetic media, and the uniformity of the probability distribution and the amplitude of the magnetization are both affected by the anisotropic parameters,²¹ which means anisotropic potential energy may also affect dielectric properties. In the above situations, eq 1 may be no longer applicable to characterize the power loss of chemical reactions. Power loss is closely related to dielectric properties, therefore, it is necessary to further study the power loss of linear reaction systems under external or internal potential energy effects.

The power loss density of electromagnetic waves in unimolecular reactions was investigated according to equivalent circuit (EC) method.²² The energy stored in a dispersed medium can be analogized to the storage of energy by inductors or capacitors in a circuit, and the energy dissipate in a dispersed medium can be analogized to the energy consumption by resistance. Ultimately, the energy dissipation process of matter can be analyzed using a circuit approach. Recently, the transient power loss with external electromagnetic waves in irreversible chemical reactions was studied in the electrodynamic (ED) method.²³ By using the electric equation of constitutive relations and combining Poynting's theorem, the energy density formula can be expressed as two terms, in which the electromagnetic energy density is the term with time derivative and the term without time derivative is the power loss. However, the interactions between polar molecules and the anisotropic potential energy are ignored, which can be usually observed in molecules.

Recently, dielectric relaxations of interacting polar molecules and uniaxial anisotropic polar molecules are studied by some researchers,^{24,25} but the power losses in these systems are not clearly. In this paper, the power losses of two kinds of molecules with linear reaction dynamics, including uniaxial anisotropic polar molecules and interacting polar molecules, are investigated in the presence of a weak external electric field by using both ED and EC methods, respectively. In Section 2, based on the modified reaction-diffusion equation, the storage power density and loss power density of the uniaxial anisotropic reacting polar molecules are derived by ED and EC methods. In Section 3, the storage power density and loss power density of interacting reacting polar molecules are further derived based on ED and EC methods. In Section 4, numerical calculations are carried out, and the results show that both the anisotropic potential energies and the interacting polar molecules have a strong impact on energy dissipation.

2. POWER LOSS IN UNIAXIAL ANISOTROPIC REACTING POLAR MOLECULES

2.1. Power Loss in Chemical Reactions by ED Method.

To simplify the analysis, an isomerization reaction is considered by assuming that the polar molecules decrease at a fixed rate and the products are nonpolar. Thus, the modified Smoluchowski-Debye equation for the probability distribution function of the molecular concentration can be expressed by²⁴

$$\frac{\partial \gamma(\theta, t)}{\partial t} = -v + \frac{D_r}{\sin \theta} \frac{\partial}{\partial \theta} \left\{ \sin \theta \left[\frac{\partial \gamma(\theta, t)}{\partial \theta} + \frac{1}{k_B T} \gamma(\theta, t) \frac{\partial V(\theta, t)}{\partial \theta} \right] \right\} \quad (2)$$

where D_r is the rotational diffusion coefficient, k_B is the Boltzmann's constant, T is the absolute temperature, θ is the

polar angle, $V(\theta, t)$ is the potential, $\gamma(\theta, t)$ is the probability distribution function, and v is the rate of $\gamma(\theta, t)$ with time, which is expressed as

$$v = -\frac{\partial \gamma(\theta, t)}{\partial t} = k\gamma(\theta, t) \quad (3)$$

where k is the rate constant.

Then, we consider an external potential energy with uniaxial anisotropy acting on the molecules²⁵

$$V(\theta, t) = -\Gamma \cos^2 \theta - \mu E(t) \cos \theta \quad (4)$$

where Γ is the uniaxial anisotropy constant of the particle, and μ is the dipole moment.

The reorientation polarization of the reacting polar molecules can be expressed as²⁴

$$P(t) = N_A \mu c(t) \frac{\int_0^\pi 2\pi \gamma(\theta, t) \cos \theta \sin \theta d\theta}{\int_0^\pi 2\pi \gamma(\theta, t) \sin \theta d\theta} \quad (5)$$

where N_A and $c(t)$ are Avogadro's number and the concentration of polar molecules, respectively.

If the probability distribution function is represented by the Legendre polynomials,²⁵ θ and t can be separated as

$$\gamma(\theta, t) = \sum_{n=0}^{\infty} \frac{2n+1}{2} A_n(t) P_n(\cos \theta) \quad (6)$$

where $P_n(\cos \theta)$ is the Legendre polynomials, and $A_n(t)$ is the corresponding coefficient of the Legendre polynomials.

Therefore, eq 5 can be simplified as

$$P(t) = N_A \mu c(t) \frac{A_1(t)}{A_0(t)} \quad (7)$$

By combining eqs 2–4 and 6, eq 2 can be represented as

$$\begin{aligned} \frac{dA_n(t)}{dt} = & -kA_n(t) + D_r \frac{\mu E(t)}{k_B T} \frac{n(n+1)}{2n+1} \\ & [A_{n-1}(t) - A_{n+1}(t)] + \frac{\sigma n(n^2-1)}{4n^2-1} A_{n-2}(t) \\ & - 2D_r \left[\frac{n(n+1)}{2} - \frac{\sigma n(n+1)}{(2n-1)(2n+3)} \right] A_n(t) \\ & - \frac{\sigma n(n+1)(n+2)}{(2n+1)(2n+3)} A_{n+2}(t) \end{aligned} \quad (8)$$

where $\sigma = \frac{\Gamma}{k_B T}$ is the dimensionless anisotropy.

Setting $n=0$ and $n=1$, we can get $A_0(t)$ and $A_1(t)$ through eq 8

$$A_0(t) = c(t) = c(0)e^{-kt} \quad (9)$$

$$\frac{dA_1(t)}{dt} + \left[k + 2D_r \left(1 - \frac{2}{5}\sigma \right) \right] A_1(t) = \frac{2}{3} \frac{\mu}{k_B T} D_r A_0(t) E(t) \quad (10)$$

where $c(0)$ is the initial concentration. Through eq 10, we get

$$\begin{aligned}
 A_1(t) &= \int_0^t \frac{2}{3} \frac{\mu}{k_B T} D_r E(t-t') A_0(t-t') e^{-[k+2D_r(1-\frac{2}{5}\sigma)]t'} dt' \\
 &= \frac{2}{3} \frac{\mu}{k_B T} D_r e^{-[k+2D_r(1-\frac{2}{5}\sigma)]t} [E(t)A_0(t)]
 \end{aligned}
 \tag{11}$$

where * represents the convolution.

By combining eqs 9 and (11), eq 7 can be represented as

$$P(t) = N_A \mu A_1(t) \tag{12}$$

According to the Poynting theorem, the dynamic equation, and Maxwell's equations, we can get the electric energy conservation equation expression^{22,26}

$$\vec{E}(t) \cdot \frac{\partial \vec{D}(t)}{\partial t} = \frac{\partial W_e(t)}{\partial t} + P_{loss}(t) \tag{13}$$

where $\vec{D}(t) = \epsilon_0 \vec{E}(t) + \vec{P}(t)$ is the electric flux density, W_e is the stored electric energy density, ϵ_0 is the dielectric constant in vacuum, and P_{loss} is the power loss. According to the expression $\vec{D}(t) = \epsilon_0 \vec{E}(t) + \vec{P}(t)$ and eq 12, eq 13 can be expressed as

$$\vec{E}(t) \cdot \frac{\partial \vec{D}(t)}{\partial t} = \frac{\partial}{\partial t} \left(\frac{1}{2} \epsilon_0 |\vec{E}(t)|^2 \right) + N_A \mu E(t) \frac{\partial}{\partial t} A_1(t) \tag{14}$$

From eq 14, it can be seen that the electric energy density will be dependent on $A_1(t)$. Taking eq 10 into eq 14, we get

$$\begin{aligned}
 \vec{E}(t) \cdot \frac{\partial \vec{D}(t)}{\partial t} &= \frac{\partial}{\partial t} \left(\frac{1}{2} \epsilon_0 |\vec{E}(t)|^2 \right) + \frac{3N_A \mu k_B T}{2\mu D_r A_0} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 \\
 &\quad + \frac{3N_A \mu k_B T}{2\mu D_r A_0} \left(k + 2D_r \left(1 - \frac{2}{5} \sigma \right) \right) \frac{\partial}{\partial t} \left(\frac{1}{2} |A_1(t)|^2 \right)
 \end{aligned}
 \tag{15}$$

By analogy with eq 13, it can be found that

$$P_{loss}(t) = \frac{3N_A k_B T}{2D_r A_0(t)} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 \tag{16}$$

$$\begin{aligned}
 \frac{\partial W_e(t)}{\partial t} &= \frac{\partial}{\partial t} \left(\frac{1}{2} \epsilon_0 |\vec{E}(t)|^2 \right) + \frac{3N_A k_B T}{2D_r A_0(t)} \\
 &\quad \left(k + 2D_r \left(1 - \frac{2}{5} \sigma \right) \right) \frac{\partial}{\partial t} \left(\frac{1}{2} |A_1(t)|^2 \right)
 \end{aligned}
 \tag{17}$$

2.2. Power Loss in Chemical Reactions by EC Method.

In the reaction system, the reactants decrease continuously and the products increase continuously until the end of the reaction process. In this situation, the classical formula in the frequency domain cannot accurately describe the power dissipation of electromagnetic waves. However, the energy conversion in this scenario is similar to that in electronic circuits, in which the resistors represent the dissipation of energy and the capacitors or inductors represent energy storage. So, we can analyze this issue using circuit methods. Being treated as an equivalent circuit by making analogies with $V \leftrightarrow E$ and $q \leftrightarrow D$, the equivalent model can be shown in Figure 1.²²

In Figure 1, d is the width between the parallel plates, A is the area of the plate, and q is the time-varying charge. On the basis of the Gauss's law, we can get

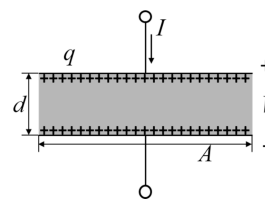


Figure 1. Model of the parallel-plate capacitor.

$$q = D(t)A \tag{18}$$

Then we can obtain the total current

$$\begin{aligned}
 I &= \frac{\partial q}{\partial t} \\
 &= A \frac{\partial \epsilon_0 E(t)}{\partial t} + A \frac{\partial P(t)}{\partial t}
 \end{aligned}
 \tag{19}$$

According to $E(t)d = V$, we can get

$$I = \frac{A\epsilon_0}{d} \frac{\partial V}{\partial t} + A \frac{\partial P}{\partial t} \tag{20}$$

Combining eqs 10 and 12 yields

$$\frac{\partial P(t)}{\partial t} + \left[k + 2D_r \left(1 - \frac{2}{5} \sigma \right) \right] P(t) = \frac{2}{3} \frac{\mu^2}{k_B T} N_A D_r A_0(t) E(t) \tag{21}$$

Taking $E(t)d = V$ into eq 21, we get

$$\begin{aligned}
 \frac{d}{\frac{2}{3} \frac{\mu^2}{k_B T} AN_A D_r A_0(t)} \frac{\partial P(t)}{\partial t} + \frac{d \left[k + 2D_r \left(1 - \frac{2}{5} \sigma \right) \right]}{\frac{2}{3} \frac{\mu^2}{k_B T} AN_A D_r A_0(t)} P(t) \\
 \int A \frac{\partial P(t)}{\partial t} = V
 \end{aligned}
 \tag{22}$$

From eqs 20 and 22, it can be seen that this equivalent circuit has two branches. One branch can be equivalent to a capacitor, as shown in the first term of eq 20, while the other branch can be equivalent to a resistor capacitor connected in series as shown in eq 22, as shown in Figure 2.

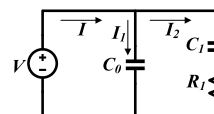


Figure 2. Equivalent circuit of the isomerization reaction.

The value of each component in Figure 2 is

$$C_0 = \frac{A\epsilon_0}{d} \tag{23}$$

$$C_1 = \frac{\frac{2}{3} \frac{\mu^2}{k_B T} AN_A D_r A_0(t)}{d \left[k + 2D_r \left(1 - \frac{2}{5} \sigma \right) \right]} \tag{24}$$

$$R_1 = \frac{d}{\frac{2}{3} \frac{\mu^2}{k_B T} AN_A D_r A_0(t)} \tag{25}$$

Only resistors consume energy in equivalent circuits, therefore, the power loss can be expressed by

$$P_{\text{loss}} = I_2^2 R_1 = \frac{Ad}{\frac{2}{3} \frac{\mu^2}{k_B T} N_A D_r A_0(t)} \left| \frac{\partial P(t)}{\partial t} \right|^2 \quad (26)$$

By applying $P(t) = N_A \mu A_1(t)$, the power loss density in this isomerization reaction is

$$P_{\text{loss}} = \frac{3N_A k_B T}{2D_r A_0(t)} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 \quad (27)$$

The total input energy can be expressed by

$$P_{\text{in}} = IV \quad (28)$$

Taking eqs 7, 11, and 19 and $E(t)d = V$ into eq 28, we get

$$P_{\text{in}} = Ad \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \varepsilon_0 |\vec{E}(t)|^2 \right) + \frac{3N_A k_B T}{2D_r A_0(t)} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 + \frac{3N_A k_B T}{2D_r A_0(t)} \left(k + 2D_r \left(1 - \frac{2}{5} \sigma \right) \right) \frac{\partial}{\partial t} \left(\frac{1}{2} |A_1(t)|^2 \right) \right] \quad (29)$$

Therefore, the power storage in this isomerization reaction is

$$\begin{aligned} \frac{\partial W_e(t)}{\partial t} &= \frac{P_{\text{in}}}{Ad} - P_{\text{loss}} \\ &= \frac{\partial}{\partial t} \left(\frac{1}{2} \varepsilon_0 |\vec{E}(t)|^2 \right) + \frac{3N_A k_B T}{2D_r A_0(t)} \left(k + 2D_r \left(1 - \frac{2}{5} \sigma \right) \right) \frac{\partial}{\partial t} \left(\frac{1}{2} |A_1(t)|^2 \right) \end{aligned} \quad (30)$$

From eqs 16 and 17 and eqs 27 and 30, we can find that the results based on the EC method and the ED method are the same. By setting $k = 0$ and $\sigma = 0$, eq 16 and eq 27 can be reduced to eq 1, which is the same as the classical formula for matter.

3. POWER LOSS IN UNIAXIALLY INTERACTING REACTING POLAR MOLECULES

3.1. Power Loss in Chemical Reactions by ED Method.

In polarized molecular reaction systems, there exists an interaction torque, which can affect the dielectric response of the system and also the power dissipation. In this section, the effect of interaction torques in a linear reaction dynamics system is studied. Similar to Section 2, the isomerization reaction is discussed, in which the reactants will be consumed at a constant rate and the products will become nonpolar molecules. Then, we consider an external potential energy with uniaxial interaction acting on the system,^{24,27} assuming that all dipole moments have the same direction and form an angle θ with the direction of the electric field,

$$V(\theta, t) = \frac{4\pi}{3} \mu P(t) \cos \theta - \mu E(t) \cos \theta \quad (31)$$

It can be seen that the first term on the right side represents the effect of interaction torques.

Taking eqs 3, 6, and 31 into eq 2, we get²⁴

$$\begin{aligned} \frac{\partial A_n(t)}{\partial t} &= -[k + n(n+1)D_r]A_n(t) \\ &+ \left[\frac{\mu E(t)}{k_B T} - \frac{4\pi N_A \mu^2}{3k_B T} \frac{c(t)A_1(t)}{A_0(t)} \right] \frac{n(n+1)}{2n+1} D_r \\ &[A_{n-1}(t) - A_{n+1}(t)] \end{aligned} \quad (32)$$

Setting $n = 0$ and $n = 1$, through eq 32, we can get $A_0(t)$ and $A_1(t)$

$$A_0(t) = c(t) = c(0)e^{-kt} \quad (33)$$

$$\begin{aligned} \frac{\partial A_1(t)}{\partial t} &= - \left(k + 2D_r + \frac{2}{3} D_r \frac{4\pi N_A \mu^2}{3k_B T} A_0(t) \right) A_1(t) \\ &+ \frac{2}{3} \frac{\mu}{k_B T} D_r A_0(t) E(t) \end{aligned} \quad (34)$$

Solving eq 34 yields

$$\begin{aligned} A_1(t) &= \frac{2D_r}{3} c(t) \int_0^t \exp \left(- \int_{t'}^t (2D_r + \frac{2D_r}{3} \frac{4\pi N_A \mu^2}{3k_B T} c(t_1)) dt_1 \right) \\ &\frac{\mu E(t')}{k_B T} dt' \end{aligned} \quad (35)$$

Taking eq 34 into eq 14, we get

$$\begin{aligned} \vec{E}(t) \frac{\partial D}{\partial t} &= \frac{\partial}{\partial t} \left(\frac{1}{2} \varepsilon_0 |\vec{E}(t)|^2 \right) + \frac{3N_A k_B T}{2D_r A_0(t)} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 \\ &+ \frac{3N_A k_B T}{2D_r A_0(t)} \left(k + 2D_r + \frac{2}{3} D_r \frac{4\pi N_A \mu^2}{3k_B T} A_0(t) \right) \frac{\partial}{\partial t} \\ &\left(\frac{1}{2} |A_1(t)|^2 \right) \end{aligned} \quad (36)$$

By analogy with eq 13, it can be found that

$$P_{\text{loss}}(t) = \frac{3N_A k_B T}{2D_r A_0(t)} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 \quad (37)$$

$$\begin{aligned} \frac{\partial W_e(t)}{\partial t} &= \frac{\partial}{\partial t} \left(\frac{1}{2} \varepsilon_0 |\vec{E}(t)|^2 \right) + \frac{3N_A k_B T}{2D_r A_0(t)} \\ &\left(k + 2D_r + \frac{2}{3} D_r \frac{4\pi N_A \mu^2}{3k_B T} A_0(t) \right) \frac{\partial}{\partial t} \left(\frac{1}{2} |A_1(t)|^2 \right) \end{aligned} \quad (38)$$

3.2. Power Loss in Chemical Reactions by EC Method.

In the above section, the power loss of interacting polar molecules with linear reaction dynamics was discussed using the ED method. Similarly, the power dissipation of this reaction system can also be analyzed using the EC method, and the analysis process is the same as that in Section 2.2.

Combining eqs 12 and (34), we get

$$\begin{aligned} \frac{\partial P(t)}{\partial t} &+ \left(k + 2D_r + \frac{2}{3} D_r \frac{4\pi N_A \mu^2}{3k_B T} A_0(t) \right) P(t) \\ &= \frac{2}{3} \frac{\mu^2}{k_B T} N_A D_r A_0(t) E(t) \end{aligned} \quad (39)$$

Similar to the derivation in Section 2.2, taking eqs 18 and 19 and $E(t)d = V$ into eq 39, we get

$$\begin{aligned} & \frac{d}{dt} \frac{A \partial P(t)}{\frac{2}{3} \frac{\mu^2}{k_B T} A N_A D_r A_0(t)} \\ & + \frac{d \left(k + 2D_r + \frac{2}{3} D_r \frac{4\pi N_A \mu^2}{3k_B T} A_0(t) \right)}{\frac{2}{3} \frac{\mu^2}{k_B T} A N_A D_r A_0(t)} \int_A \frac{\partial P(t)}{dt} \\ & = V \end{aligned} \quad (40)$$

The equivalent circuit is the same as that in Figure 2. Due to the interaction between the molecules, the value of each component in Figure 2 will be different from that in Section 2.2, which is given by

$$C_0 = \frac{A \varepsilon_0}{d} \quad (41)$$

$$C_1 = \frac{\frac{2}{3} \frac{\mu^2}{k_B T} A N_A D_r A_0(t)}{d \left(k + 2D_r + \frac{2}{3} D_r \frac{4\pi N_A \mu^2}{3k_B T} A_0(t) \right)} \quad (42)$$

$$R_1 = \frac{d}{\frac{2}{3} \frac{\mu^2}{k_B T} A N_A D_r A_0(t)} \quad (43)$$

Only resistors consume energy in equivalent circuits, we can get the power loss density in this reaction

$$P_{\text{loss}} = \frac{3N_A k_B T}{2D_r A_0(t)} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 \quad (44)$$

Taking eqs 7, 19, and 35 and $E(t)d = V$ into eq 28, we get

$$\begin{aligned} P_{\text{in}} = Ad & \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \varepsilon_0 |\vec{E}(t)|^2 \right) + \frac{3N_A k_B T}{2D_r A_0(t)} \left(\frac{\partial A_1(t)}{\partial t} \right)^2 \right. \\ & + \frac{3N_A k_B T \left(k + 2D_r + \frac{2}{3} D_r \frac{4\pi N_A \mu^2}{3k_B T} A_0(t) \right)}{2D_r A_0(t)} \frac{\partial}{\partial t} \\ & \left. \left(\frac{1}{2} |A_1(t)|^2 \right) \right] \end{aligned} \quad (45)$$

Therefore, the power storage is

$$\begin{aligned} \frac{\partial W_e(t)}{\partial t} &= \frac{P_{\text{in}}}{Ad} - P_{\text{loss}} \\ &= \frac{\partial}{\partial t} \left(\frac{1}{2} \varepsilon_0 |\vec{E}(t)|^2 \right) + \frac{3N_A k_B T}{2D_r A_0(t)} \\ & \left(k + 2D_r + \frac{2}{3} D_r \frac{4\pi N_A \mu^2}{3k_B T} A_0(t) \right) \frac{\partial}{\partial t} \\ & \left(\frac{1}{2} |A_1(t)|^2 \right) \end{aligned} \quad (46)$$

From eqs 37 and 38 and eqs 44 and 46, we find that the results through the EC method and the ED method are also the same.

By setting $k = 0$ and ignoring the interaction torques terms, eq 37 and eq 44 can be reduced to eq 1.

4. RESULTS AND DISCUSSION

In Sections 2 and 3, the expressions of power loss with linear reaction dynamics by considering the influence of anisotropic potential energy and interaction torques are derived using both ED and EC methods. In addition, the reaction processes of both situations are assumed to be equilibrium before $t = 0$ and begin at $t = 0$, then we can get the power loss of both situations. From eq 11, we have

$$A_1(t) = \frac{2u_0 c(0) D_r}{3} \frac{e^{-kt} \left[2D_r \left(1 - \frac{2}{5} \sigma \right) \cos \omega t + \omega \sin \omega t \right] - 2D_r \left(1 - \frac{2}{5} \sigma \right) e^{-[k+2D_r(1-\frac{2}{5}\sigma)]t}}{\left[2D_r \left(1 - \frac{2}{5} \sigma \right) \right]^2 + \omega^2} \quad (47)$$

where $u_0 = \frac{\mu E_0}{k_B T}$, $E(t) = E_0 \cos(\omega t)$, and E_0 is the amplitude of the

electric field.

The power loss in the anisotropic reacting system can be

expressed as, based on eq 16,

$$\begin{aligned}
 P_{\text{loss}} &= \frac{3N_A k_B T}{2D_r A_0(t)} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 \\
 &= \frac{2D_r N_A k_B T c(0) u_0^2 e^{kt}}{3} \left| \frac{e^{-kt} \left[-2D_r \left(1 - \frac{2}{5}\sigma\right) k + \omega^2 \right] \cos \omega t}{\left[2D_r \left(1 - \frac{2}{5}\sigma\right) \right]^2 + \omega^2} \right. \right. \\
 &\quad \left. \left. - \frac{e^{-kt} \left[k + 2D_r \left(1 - \frac{2}{5}\sigma\right) \right] \omega \sin \omega t}{\left[2D_r \left(1 - \frac{2}{5}\sigma\right) \right]^2 + \omega^2} \right. \right. \\
 &\quad \left. \left. + \frac{2D_r \left(1 - \frac{2}{5}\sigma\right) e^{-kt} \left[k + 2D_r \left(1 - \frac{2}{5}\sigma\right) \right] e^{-2D_r \left(1 - \frac{2}{5}\sigma\right) t}}{\left[2D_r \left(1 - \frac{2}{5}\sigma\right) \right]^2 + \omega^2} \right|^2 \quad (48)
 \end{aligned}$$

Similarly, we can get the power loss in the interacting system

based on eq 37 by expanding the exponential in the integral of eq

35 with Taylor's series, which is given by

$$\begin{aligned}
 A_1(t) &= \frac{2D_r}{3} c(t) \int_0^t \exp\left(-\int_{t'}^t (2D_r + \frac{2D_r}{3} \frac{4\pi N_A \mu^2}{3k_B T} c(t_1) dt_1)\right) \\
 &\quad \left. \frac{\mu E(t')}{k_B T} dt' \right. \\
 &= \frac{2D_r c(0) u_0 e^{-kt}}{3} \left\{ \left[1 + \frac{2D_r \lambda c(0) e^{-kt}}{3k} \right] \right. \\
 &\quad \left. \frac{2D_r \cos \omega t + \omega \sin \omega t - 2D_r e^{-2D_r t}}{\omega^2 + (2D_r)^2} \right. \\
 &\quad \left. - \frac{2D_r \lambda c(0) e^{-kt}}{3k} \right. \\
 &\quad \left. \frac{(2D_r - k) \cos \omega t + \omega \sin \omega t - (2D_r - k) e^{-(2D_r - k)t}}{\omega^2 + (2D_r - k)^2} \right\} \quad (49)
 \end{aligned}$$

where $\lambda = \frac{4\pi N_A \mu^2}{3k_B T}$.

Then, eq 37 can be expressed as

$$\begin{aligned}
 P_{\text{loss}} &= \frac{3N_A k_B T}{2D_r A_0(t)} \left| \frac{\partial A_1(t)}{\partial t} \right|^2 \\
 &= \frac{2D_r N_A k_B T c(0) u_0^2 e^{kt}}{3} \left| \left[-ke^{-kt} - \frac{4D_r c(0) \lambda e^{-2kt}}{3} \right] \right. \\
 &\quad \left. \frac{2D_r \cos \omega t + \omega \sin \omega t - 2D_r e^{-2D_r t}}{\omega^2 + (2D_r)^2} \right. \\
 &\quad \left. + \left[e^{-kt} + \frac{2D_r c(0) \lambda e^{-2kt}}{3k} \right] \right. \\
 &\quad \left. \frac{-2D_r \omega \sin \omega t + \omega^2 \cos \omega t + (2D_r)^2 e^{-2D_r t}}{\omega^2 + (2D_r)^2} \right. \\
 &\quad \left. + \frac{4D_r c(0) \lambda}{3} e^{-2kt} \right. \\
 &\quad \left. \frac{(2D_r - k) \cos \omega t + \omega \sin \omega t - (2D_r - k) e^{-(2D_r - k)t}}{\omega^2 + (2D_r - k)^2} \right. \\
 &\quad \left. - \frac{2D_r c(0) \lambda}{3k} e^{-2kt} \right. \\
 &\quad \left. \frac{-(2D_r - k) \omega \sin \omega t + \omega^2 \cos \omega t + (2D_r - k)^2 e^{-(2D_r - k)t}}{\omega^2 + (2D_r - k)^2} \right|^2 \quad (50)
 \end{aligned}$$

To understand the power losses in the two scenarios, numerical calculations are needed. In Figure 3, the power losses in anisotropic system with different anisotropic potential energies and different reaction rates are both shown at various time according to eq 48. The parameters in these expressions are

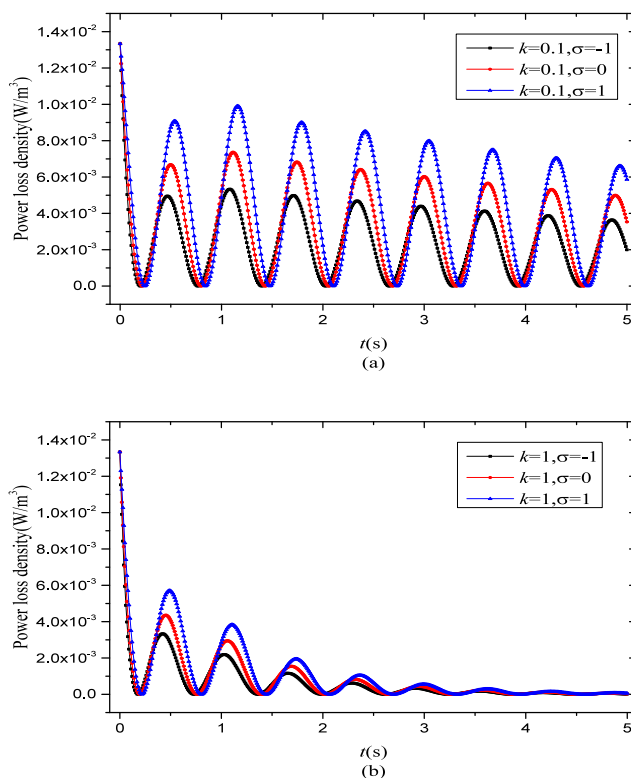


Figure 3. Total power loss density in anisotropic system with different reaction rates: (a) $k = 0.1$, (b) $k = 1$.

set based on the numerical values in ref 24, and the results are normalized by $N_A k_B T c(0)$. It is assumed that $u_0 = 0.1$, $D_r = 2$, $\omega = 5$, the reaction rate constant k is 0.1 and 1, different numerical calculations based on $\sigma = -1, 0$, and 1 are obtained and compared. As shown in Figure 3(a), the reaction rate constant k is 0.1, it can be seen that the influence of anisotropic potential energies on power loss is very obvious. The power loss of case $k = 0.1$, $\sigma = -1$ decreases about 27% at each peak compared to case $k = 0.1$, $\sigma = 0$. In the case of $k = 1$, the power loss decreases about 24%, obviously the power loss is suppressed, the decrease in power loss after an increase in reaction rate is mainly attributed to a higher consumption of reactants. In the case of $\sigma = 1$, the power loss has increased about 32% ($k = 0.1$) and 27% ($k = 1$), which means anisotropic potential energy promotes power loss. Meanwhile, as shown in Figure 3(b), when the reaction rate k increases to 1, the power loss will be reduced to 0 at about 4 s, since the reactants have been completely consumed.

In Figure 4, the power losses of interacting system under different conditions and time are presented based on eq 50,

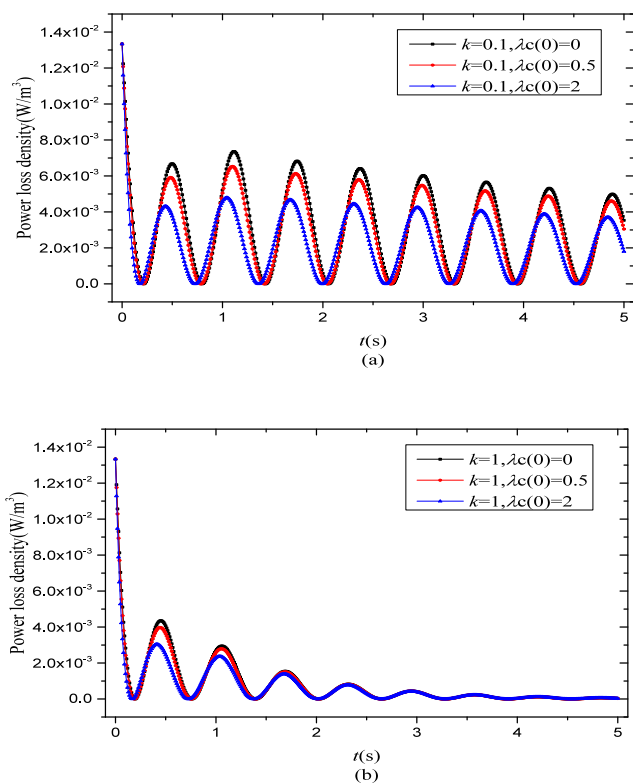


Figure 4. Power loss density in interacting system with different reaction rates: (a) $k = 0.1$, (b) $k = 1$.

which are also normalized by $N_A k_B T c(0)$. It is assumed that $u_0 = 0.1$, $D_r = 2$, $\omega = 5$, the reaction rate k is 0.1 and 1, different numerical calculations based on $\lambda c(0) = 0, 0.5$, and 2 are obtained and compared. When the reaction rate k is 0.1, in Figure 4(a) we can find that the interacting torque has a significant impact on the system. The one without interacting torque has the maximum power loss, and the power loss decreases about 10% ($\lambda c(0) = 0.5$) and 30% ($\lambda c(0) = 2$). When the reaction rate k is 1, as shown in Figure 4(b), there is no significant difference in power loss after $t = 1.5$ s and the power loss is reduced to 0 at about 4 s because the reactants have been depleted, which has the same trend as that in Figure 3(b). By Comparing Figure 3 and Figure 4, we can also find that the case

in Figure 3 with $\sigma = 0$ has the same power loss with the case $\lambda c(0) = 0$ in Figure 4, since only chemical reaction process is considered and the influence of other factors is ignored in both cases.

It is worthy of note that the power loss density at the first peak (at about time $t = 0.5$) is lower than that at the second peak (at about time $t = 1$) in both Figure 3(a) and Figure 4(a), which seems to be abnormal because power loss density will decrease with the consumption of reactants. To find the reason, we need to clarify the relationship among three time periods, the relaxation time of dipole rotation $\tau = 1/(2D_r)$, the microwave cycle $t_m = 2\pi/\omega$, and the reaction time $t_{ch} = 1/k$. In Figure 3(a) and Figure 4(a), these three parameters are $\tau = 0.25$, $t_m \approx 1.25664$, and $t_{ch} = 10$, which means the relaxation time of dipole rotation is comparable with half a microwave cycle. That is to say the orientation polarization is inadequate in half a microwave cycle, leading to the lower power loss at the first peak. The power losses are discussed by changing the angular frequency, as shown in Figure 5. It can be seen that when ω decreases, the power loss

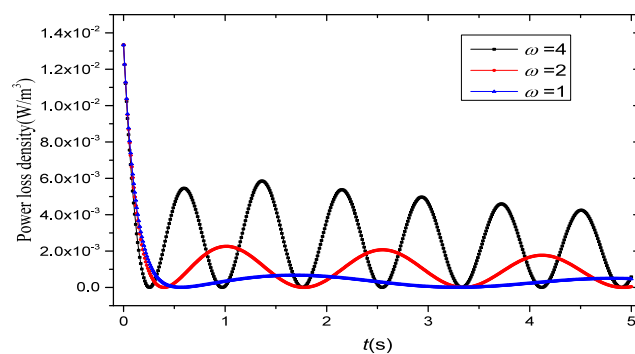


Figure 5. Power loss density in reaction system when $u_0 = 0.1$, $D_r = 2$, $k = 0.1$ (Normalized by $N_A k_B T c(0)$).

density will decrease with time continuously like a damped oscillation, since the microwave cycle will increase as ω decreases, which gives rise to adequate orientation polarization in the first microwave cycle. On the other hand, for $k = 1$, the reaction time will be 1 s, and the three parameters will be comparable with each other. However, the chemical reaction process will be dominant in the energy dissipation since the reactants decrease exponentially, as shown in Figure 3(b) and Figure 4(b).

From the above results, it can be found that the power loss of linear reaction systems is directly related to dielectric characterization. In ref 28, experimental results are consistent with those of previous studies in refs 18, 22, and 24, and the power loss of the paper is also calculated based on these theories, which shows that the research results may be reliable.

5. CONCLUSIONS

In this paper, the general expressions of power losses in two polar-molecule isomerization reaction systems, including the anisotropic system and the interacting system, are derived based on both ED method and EC method. It can be seen that the results obtained by the two methods are consistent. The anisotropic potential energies have a significant impact on overall power loss. When $\sigma = 1$, power dissipation is enhanced, and the power dissipation is weakened when $\sigma = -1$. Furthermore, when the reaction rate is larger, the power loss quickly drops to nearly zero due to the depletion of reactants. In

the interacting system, the interaction energy also decreases the power loss. The greater the interaction potential energy between particles, the smaller the power loss can be found. When the reaction rate is increased, the power loss will also quickly decrease due to the end of the reaction process. In both cases, when ω decreases, the power loss density will continuously decrease over time like a damping oscillation.

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Notes

The authors declare no competing financial interest.

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