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Research Paper

Understanding of electro-conjugate fluid flow with dibutyl decanedioate using numerical simulation—Calculating ion mobility using molecular dynamics simulation

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ABSTRACT

An electro-conjugate fluid (ECF) is a type of dielectric functional fluid, which generates a powerful flow when a high direct-current voltage is applied. To date, ECF flow has been used in mechanical, chemical and biomedical applications because of its outstanding properties as a micro-pressure source for compact fluid-driven systems. However, the mechanism of ECF flow generation is not clarified and a basic understanding of ECF flow is required to progress ECF applications. We have developed the basic understanding of ECF flow generation through mathematical modeling, and have investigated electrical parameters theoretically. We have clarified microscopically the mechanism for ECF flow generation. We have proven the adequacy of the developed basic understanding by comparing visualized and computed flow characteristics. Furthermore, we have clarified the mechanism for ECF flow generation by comparing ionic transfer and ECF flow.

1. Introduction

An electro-conjugate fluid (ECF) is a type of dielectric fluid that generates a powerful flow when a high direct-current (DC) voltage is applied [1]. According to the previous study, an ECF is characterized by its conductivity vs. viscosity relation [2]. The phenomenon of generating a flow under an applied voltage, is termed an electrohydrodynamics (EHD) phenomena [3–5]. ECF flow is categorized as a type of EHD flow. However, ECF produces a much stronger flow than previously reported EHD flows [6]. Consequently, ECF flow has been used as a micropressure source for compact fluid-driven systems. Because of its outstanding properties as a micropressure source, ECF flow has been applied to many fields, including mechanical, chemical and biomedical applications, such as ECF micromotors [7], ECF micro-artificial muscles [8] and droplet-based micro-total-analysis systems [9]. However, the principle of ECF flow generation remains an open research problem, because the above-mentioned ECF applications have been developed through trial and error. To progress ECF applications, a basic understanding of ECF flow is required. Previous research suggests that an electric force is the governing force in ECF flow generation [10], however, the electric parameters, e.g. dominant ion and ion mobility, required to calculate electric forces are not obtained theoretically, and the biggest problem is to clarify the mechanism of ECF flow generation.

To solve this problem, we derive unknown electric parameters experimentally and by calculation using a molecular dynamics (MD) simulation. We perform a computational fluid dynamics (CFD) simulation based on mathematical model embedding of the obtained electric parameters. Finally, we validate the ECF flow model by comparing the visualized flow with the computed flow, and clarify the mechanism for ECF flow generation by comparing ionic transfer with ECF flow.

2. Materials and methods

2.1. Electrically induced flow in ECF

Of the numerous fluids that can be categorized as ECFs [2], we selected dibutyl decanedioate (DBD, New Technology Management Co., Ltd., Tokyo, Japan) as a working fluid. The physical properties of DBD at the experimental temperature of 293.15 K are shown in Table 1. We could not observe the induced DBD flow, because DBD

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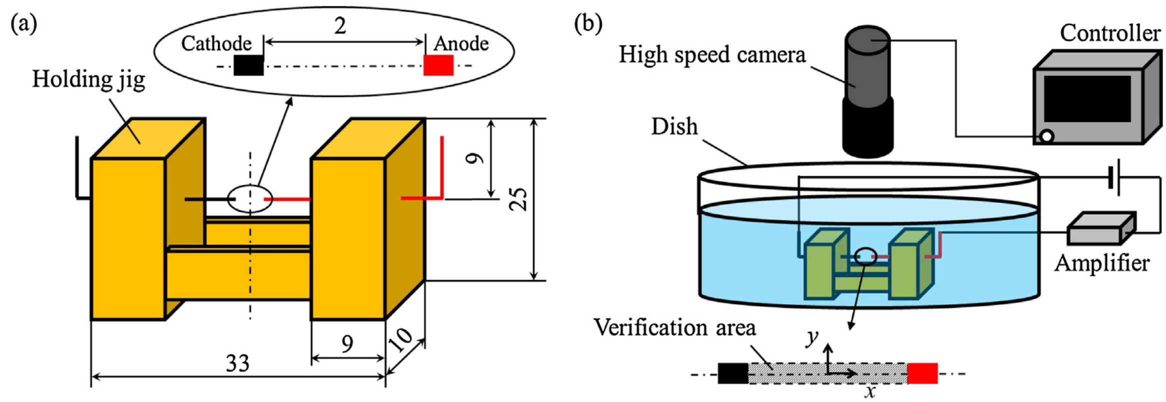

Fig. 1. Experimental setup for flow visualization. (a) Symmetrically facing stainless-steel wire electrodes, (b) visualization setup for the ECF flow.

Table 1
Physical properties of DBD at 293.15 K.

Relative permittivity [−]	Conductivity [S/m]	Density [kg/m^3]	Viscosity [Pa s]
4.8	6.8×10^{-10}	938	7.5×10^{-3}

is a transparent liquid. We obtained the flow velocity distribution by using a particle-image-velocimetry (PIV) technique [11].

ECF flow was generated by applying a DC voltage to symmetrically facing stainless-steel wire electrodes shown in Fig. 1(a). The stainless steel wire electrodes (ϕ 0.3 mm) were cut by using a precision cutting machine to obtain smooth end faces with sharp edges. The electrode gap was maintained by a holding jig made of polyether imide, which has electric insulation and a corrosion resistance against DBD. The electrode gap was 2.0 mm. The symmetrically facing electrodes were placed in a dish (ϕ 58 mm), and the DBD that was mixed with tracer particles (MBX-12, Sekisui Plastics Co., Ltd., Tokyo, Japan) was added to the dish as shown in Fig. 1(b). The voltage that was applied to the electrodes was between 0 kV and 3.0 kV with a DC power supply (PW18-2ATP, KENWOOD, Tokyo, Japan) and a voltage amplifier (HV-10P, Matsusada Precision, Shiga, Japan). The focus plane of a high-speed camera (HV-100C, KEYENCE, Osaka, Japan) was set at the center of the electrodes and the flow was recorded for 2.5 s after a step input had been applied. The flow was recorded by a high-speed camera controller (VW-6000, KEYENCE, Osaka, Japan), and the flow distribution was obtained by using PIV software (PIVlab 1.4, William Thielicke, Bremen, Germany). The verification area was defined relative to the interelectrode area as shown in Fig. 1(b).

2.2. Modeling of ECF flow

Previous research suggests that the electric force is a governing force for ECF flow generation, because ECF flow is generated by applying a voltage [10]. The electric body force $\boldsymbol{F_v}$ that works on the dielectric fluid is given as:

$$\boldsymbol{F_v} = q\boldsymbol{E} - \frac{\varepsilon_0}{2}E^2\nabla\varepsilon_r + \frac{\varepsilon_0}{2}\nabla\left(E^2\frac{\partial\varepsilon_r}{\partial\rho}\rho\right) \quad (1)$$

where q is the charge density, ρ is the fluid density, $\boldsymbol{E}$ is the electric field, ε_0 is the permittivity of vacuum and ε_r is the relative permittivity. From Eq. (1), the electric force that acts on a dielectric fluid is classified into three types; the Coulomb force, the dielectric force and the electrostriction force. However, if we consider that DBD is a pure liquid and that the flow is incompressible, the governing force for flow generation may be the Coulomb force only. By inserting this information into the Navier–Stokes equation, the equation of motion for the ECF flow is given as:

$$\frac{\partial\boldsymbol{u}}{\partial t} = -(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} - \frac{1}{\rho}\nabla p + \frac{\eta}{\rho}\nabla^2\boldsymbol{u} + \frac{1}{\rho}q\boldsymbol{E} \quad (2)$$

where $\boldsymbol{u}$ is the flow velocity, p is the pressure and η is the viscosity. Therefore, according to Eq. (2), we can understand the ECF flow by investigating the Coulomb force that is induced by the electric field and charges.

Because the charge density between the electrodes is constant (see Supplementary Note 1), the electric-potential distribution in DBD is given as:

$$\nabla^2 V = \frac{q}{\varepsilon_0\varepsilon_r} \quad (3)$$

where V is the electric potential. The electric-field distribution can be calculated by using the electric-potential distribution from Eq. (3):

$$E = -\nabla V \quad (4)$$

Ions in a dielectric fluid are moved due to the electric field, the flow velocity and the diffusion of charge [3]. Therefore, the current density in a dielectric fluid is calculated as:

$$\boldsymbol{j} = q\mu_I\boldsymbol{E} + q\boldsymbol{u} - D\nabla q \quad (5)$$

where $\boldsymbol{j}$ is the current density, μ_I is the ion mobility and D is the charge diffusion coefficient. The transport equations of charge are calculated as:

$$\frac{\partial\boldsymbol{q}}{\partial t} = -\nabla(q\mu_I\boldsymbol{E} + q\boldsymbol{u} - D\nabla q) \quad (6)$$

However, because the electric field at the electrode surface may have a threshold value to make DBD flow [12,13], the charge density is calculated as:

$$q = k(E_{static} - E_{thres}) \quad (7)$$

where k is the proportional constant for injected charge density, E_{static} is the electric field of the electrode surface and E_{thres} is the threshold value of the electric field of the electrode surface to flow generation.

2.2.1. Dominant ion

A dominant ion polarity exists in a dielectric liquid when a high voltage is applied [10], which may influence the direction of the ECF flow. The dominant ion polarity can be clarified by observing the Sumoto effect [14], in which the fluid surface rises along the rod electrodes that are inserted vertically against a dielectric liquid surface when the voltage is applied as shown in Fig. 2. Because there