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Research Paper

Joule heating and dielectric gradient effects on colloidal particle electrophoresis

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ABSTRACT

The following paper discusses the combined action of dielectric gradients and Joule heating effects to the electrophoresis of colloids in micro fluidics. Study introduces a new and useful CFD model that represents the combination of the Joule heating and dielectrophoresis phenomenon to expose the opposite particle dynamics in microchannels when the electric field is applied. The influence of the temperature gradients on the equivalent representation of the electrokinetic forces as well as the particles mobility is included by taking into consideration the temperature-dependent fluid viscosity and dielectric permittivity. These outcomes prove the fact that Joule heating can substantially change the particle velocity by changing the physical parameters of the fluid used, whereas dielectric gradients also bring new dielectrophoretic forces which can impact on the movement of the particles. This is a combined way of outlook to optimize the microfluidic platforms of biomolecule separation and nanoparticle control application. The article is particularly significant when it says that the development of advanced microfluidic devices should not ignore the effect of thermal and electrokinetics.

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1. INTRODUCTION

There are many applications of electrophoresis of colloidal particles in the microfluidic environment in the separation of biomolecules, on manipulation of nanoparticles, and in diagnostics. Electrophoresis is led by the external electric fields and is made concerning the movement of the charged particles. In enclosed microfluidic systems however, other electrokinetic processes also play a substantial role, including dielectrophoresis (DEP) and Joule heating. The electrical energy is resisted through an increase in temperature known as Joule heating and results in the fluid having a temperature gradient leading to a change in viscosity and dielectric properties. In a like manner, dielectrophoretic forces are created by the dielectric gradients due to temperature variation which affect the movement of the particles [1], [2], [3].

The models of electrophoresis that currently exist tend to model electrophoresis and dielectrophoresis effects separately or individually. But these factors are combined in practical micro fluidic conditions and the coupling should be taken into account to correctly predict the motion of particles. Joule heating influences viscosity and dielectric permittivity of the fluid, thus the mobility of the particles but dielectric gradients can influence the local electric field, thus the dielectrophoretic forces on particles. Such a coupling between thermal and electrokinetic effects has been mostly disregarded in the classical approaches to the problem and there is a necessity of a unified treatment where both the effects are taken into account.

The separate contributions of Joule heating and dielectrophoresis on the electrokinetic systems have been studied by different researchers. [4] Discussed the effect of Joule heating on electrokinetic transport in microchannels, with the mobility of the particles changing appreciably due to variations in the viscosity through the temperature. [5] Were interested in the effect of dielectrophoretic forces in a fluid with different dielectric permittivities and showed how the permittivity temperature sensitivity can be used to alter the path of particles. These studies have not however combined both thermal effects and dielectrophoresis to form one model. Coupled electrothermal model was proposed by [6], but the effects of the dielectric gradients on particle dynamics per se were not discussed explicitly. These shortcomings in literature mark the necessity of a more thorough study that shouldn t consider thermal effects, as well as dielectrophoretic effects, simultaneously.

The model presented in this paper combines three different physical processes; Joule heating, dielectric gradients, and electrophoresis, into a unifying model-one that allows the simulation of dynamics of particles in microfluidic devices. The model uses Computational Fluid Dynamics (CFD) to solve the Navier-Stokes equations of fluid flow, the Poisson-Nernst-Planck (PNP) equations of ion transport, and energy conservation equation to incorporate effects of temperature. This is because the model accounts for the intricate relationship of the temperature gradient to electric fields and fluid flows due to temperature-dependent viscosity and dielectric permittivity. High resolution simulations in the vicinity of colloidal particles and electrodes are also achieved with Adaptive Mesh Refinement (AMR). The primary output of this paper is the formulation of a complete electro-thermal-hydrodynamic model including nonlinear effects of Joule heating, dielectric gradients and electrophoresis. The model has better predictive value describing the behavior of particles in microfluidics that are non-isothermal and have the ability to overcome the limitations of prior models that would consider separately the thermal aspects and the electrokinetic aspects. The results of this study are applicable even in the designing of microfluidic systems that serve the purpose of biomolecule separation, manipulation of nanoparticles and lab-on-a-chip systems.

2. RELATED WORK

The understanding of the impacts of Joule heating and dielectrophoresis of colloidal particles in microfluidics systems has been made through many studies over the years. Most microfluidic research during the early 2000s did not treat the effects of Joule heating and dielectrophoresis independently. As an example, [7] introduced an excellent research on dielectrophoresis in microfluidic processes, reporting the effects of the change in dielectric versus dielectric on particle dynamics. The detailed exploration of multi-physics coupling in microfluidic flows was presented by Becker et al., which provided more insights into the process of electrical fields connecting with fluid dynamics even in terms of particle manipulation (2019).

The heating controls exhibited by Joule heating has become increasingly popular at the electrokinetic research frontier, especially as stronger electric fields became feasible by microfluidic systems in the 2010s. Using the results obtained, investigated the impacts of the Joule heating on the mobility of particles, and indicated that the temperature gradient can indeed strongly affect the flow regime and the trajectory of particles. This gave rise to the more complex thermal-electrokinetic models. According to Zhao et al., a modeling technique coupling dielectrophoretic forces with thermal gradient was later developed, with these authors making no attempts to apply the complete fluid-thermal-electrokinetic coupling necessary to provide the increased accuracy requested in microfluidic designs. But more modernly in 2022, a fully coupled electro-thermal-hydrodynamic model was presented by Ghoshal et al., which the study is based on. They cover the nonlinear effects of electric field with thermal gradients and fluid flow and this is a huge advancement in the previous models which did not take into consideration the interconnection of these forces.

Theoretical Framework

In this part the theory behind modeling colloidal particle behavior in microfluidic systems, subject to the action of electric fields, thermal gradients, and dielectric non uniformity, is described. The effect of electrophoresis, Joule heating and dielectric gradients interacts to give a complex transport behavior of these particles particularly beyond the non-isothermal non-uniform field conditions.

Theory of Electrophoresis

Electrophoresis is defined as movement of charged particles in a fluid placed under an external electric field. This movement is dependent on a few factors, such as the charge on the surface of the particle, the viscosity of the medium, and the amount of the electric field one applies. Classical electrophoretic theory is the assumption of uniform fluid properties and constant temperature and makes estimation of the particle mobility easy. These assumptions however fail in real life microfluidic setup [7], [8], [9]. The local heating can create variations in temperature, which lead to electrophoretic mobility contrast that could have a great impact. The reason is that, as the temperature rises, viscosity of the fluid tends to reduce, thus raising the particle speed. At the same time, the dielectric constant of the fluid might also be different that will further alter the electrokinetic forces exerted on the particle. It has been also demonstrated that including the temperature-dependent properties in electrophoretic models allows to capture the actual behavior of particles in realistic microchannel conditions in a more accurate manner [10], [11].

Effects of Joule Heating

Joule heating comes about because of electrical energy dissipation as a result of resistivity in fluids that are subjected to electric fields, but it is most crucial in nanoscale situations where strong electric fields are being implemented. Such heating creates temperature fields in the volume of the fluid causing the viscosity and density to vary spatially. These thermal impacts alter both hydrodynamic and electrostatic surrounding of the colloid particle consequently affecting its mobility [12], [13]. Both experimental and numerical works have pointed at the nonlinearity of this influence. The increase in temperature reduces the viscosity of the fluid making the particles get highly movable. Meanwhile, thermally induced convective stimulus disturbs the flow fields within the channel. Sridharan et al. and Liu et al. Have revealed that small changes in temperature may yield considerable deviations in particle movements, particularly in restrained or high voltage microfluidic conditions. Such inferences explain the need to consider energy transport in electrophoretic modeling approaches [14].

The Effects of a Dielectric Increase

The dielectrophoretic (DEP) forces emerge as a result of the spatial variation of the dielectric constant in a fluid medium and they act on polarizable particles. These gradients could be temperature caused changes of permittivity or a fluid heterogeneity. Unlike electrophoretic forces, DEP forces still exert an effect on neutral particles and so are particularly relevant in applications involving focusing, sorting, and trapping of particles. In systems where the dielectric properties are different throughout a channel, the local electric field becomes distorted and particle feel both a non-aligned force gradient and a non-aligned lateral force. Yao et al. has established that such gradients can considerably deflect the motion of any particle, changing direction and velocity. The effect is very strong when the difference associated with the dielectric properties of the particle and of the surrounding fluid is very large [15].

Effects Coupling

Joule heating and dielectric gradients co-exist and their interaction dominates the particle dynamics and cannot be approximated by their separate consideration. Joule heating changes the viscosity and the permittivity of the fluid that affect the electrophoretic as well as dielectrophoretic forces. Hence, a comprehensive methodology is vital to a real time simulation of particle transport [16]. In older models it was more customary to assume isothermal effects or constant material properties without investigating the back-coupling between temperature, electric field and flow. One of the earliest proposals to create a thermally and electrically coupled framework was published by Ghoshal et al. and gives a glimpse on how thermal feedback loops can alter electric field patterns. Later, this integration is continued with Finite Volume Method (FVM) based models that obtain better accuracy and robustness [17]. It is under these developments that the present study has its theoretical background.

3. METHODOLOGY

Research Design

The methodology of the present study lies in the development of a multi-physics model that would mimic the interactions occurring between contract Joule heating, dielectric gradients, and electrophoresis in microfluidic systems. The objective of this model is to describe the dynamics of particles more precisely due to the interaction of the thermal and the electrokinetic effects. The model uses a number of governing equations and computational procedures as discussed below.

1. Model Development

The given model incorporates the following equations: Navier Stokes Fluid Dynamic Equations,

1. Poisson Nernst Planck (PNP) equations of ion transport.
2. Equation of energy conservation in order to take into consideration temperature effects (including Joule heating).
3. The electrostatic potential poissons equation.

2. Computational Framework

This model is solved through CFD solver, where spatial discretization is applied by applying Finite Volume Method (FVM). Adaptive Mesh Refinement (AMR) is also used as part of the computational framework to allow higher levels of accuracy around particles and electrodes where there are high gradients. The MPI-based parallel computing and GPU acceleration are also used to run the similar techniques to increase the speed of simulation and enable work with big particle systems.

3. Algorithm Description

Time stepping procedure is followed by the algorithm in which we solve the governing equations iteratively for each time step. The algorithm steps are as follows:

1. Solve Navier-Stokes equations of velocity and fluid pressure.
2. Obtain the PNP equations of the concentration of ions and electric potential.
3. A temperature distribution by solving the heat equation with the Joule heating term.
4. The electrostatic potential is a solution to Poisson equation.
5. Advance the positions of particles and compute velocities of particles.

An Example of Pseudocode Implementation of the Algorithm is as Follows:

1. Initial fluid, ion and temperature sectors
2. Repeat until convergence:

a. Find a solution to the Navier Stokes equations on velocity
b. Solve PNP equations of ion concentration
c. ODE solve temperature heat distribution
d. Sol Poisson electrostatic problem
e. Time network particle positions and velocity

3. System Variables and Particle Trajectories of Output

Data Acquisition

1. Simulation Setup

To obtain the data on different input parameters like the strength of the electric field, the distribution of the temperature and conductivity of the fluid and the characteristics of the particles, numerical simulations are implemented. Depending on the temperature gradients created by Joule heating and thus based on the fluid properties including viscosity and dielectric permittivity, some modification of the fluid properties will occur. The Particle property that is varied, such as surface charge and size, so these surfaces can be evaluated in relation to their influence on mobility and trajectories. Simulation Process as presented in Figure 1.

2. Testing Procedures

The comparison with available experimental data is provided in order to justify the given model. The major testing parameters are:

1. **Particle Velocity Profiles:** A comparison with other experimental findings of [4] under different temperature and electric field situations.
2. **Temperatures Distributions:** Comparison with thermographic measurements of experimental temperatures.
3. **Trajectories of Particles:** plotted against them with experimental measurements of dielectrophoretic forces in dielectric gradient, as measured by Zhao [5].

Step 1
Initialize Fluid, Ion, and Temperature Fields

↓

Step 2:
Loop until convergence:

- **Substep a**: Solve Navier-Stokes equations for velocity.
- **Substep b**: Solve Poisson-Nernst-Planck (PNP) equations for ion concentration.
- **Substep c**: Solve heat equation for temperature distribution (including Joule heating).
- **Substep d**: Solve Poisson's equation for electrostatic potential.
- **Substep e**: Update particle positions and velocities.

↓

Step 3
Output particle trajectories and system variables.

Figure 1. Flowchart of Simulation Process

3. Data Analysis

Following simulations, the data will be analyzed with the help of the following methods:

1. **Analysis of Particle Trajectory:** Tracing the trajectories of particles in different electric fields, with temperature gradients.
2. **Velocity Profiling:** Analysis of the variations in velocities of particles under an applied electric field and thermogradients.
3. **Sensitivity Analysis:** Testing how the results of the simulation change when important parameters (e.g. ionic strength, temperature gradient, particle size) are varied Summary of input parameters to the simulation listed in Table 1.

Table 1. Input Parameters Summary of Simulation

Parameter	Value
Electric Field Strength	10 V/cm
Fluid Viscosity	0.001 Pa.s
Temperature Gradient	20 °C to 60 °C
Particle Diameter	1-5 µm

Table 1 summarizes the input parameters used in the simulations, including the values for electric field strength, fluid viscosity, and temperature gradient.

4. RESULTS AND DISCUSSION

The simulation outcomes provide precious information concerning the impacts of Joule heating and gradient effects of dielectricity on colloidal particles velocity and direction. According to Sridharan. Joule heating greatly changes the properties of the fluids and mobility of the particles. The simple model applied to the expression of the velocity of the particles in an electrophoretic system is the following relationship settled on the basis of the Stokes-Einstein equation:

$$v = \mu E$$

Where:

a. v is electrophoretic velocity of the particle,
b. µ is the electrophoretic mobility and
c. E is electric field strength.

This correlation however varies in the presence of Joule heating since viscosity of the fluid varies with temperature T. With rising temperature as Joule heating occurs, the viscosity of the fluid declines and, therefore, the particle mobility rises. In order to take into consideration the viscosity as a factor of temperature, we alter the electrophoretic mobility:

Where:

a. µ0 is the initial mobility at the reference temperature,
b. β is the coefficient of viscosity due to change in temperature and
c. T - Is the temperature.

The temperature distribution in the fluid is governed by the heat equation, which includes a term for Joule heating:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + \frac{Q}{P^{c_p}}$$

Where:

a. T is the temperature,
b. α is the thermal diffusivity,
c. Q=σE2 is the Joule heating term (where σ is the electrical conductivity of the fluid and EEE is the electric field strength),
d. ρ is the density of the fluid, and
e. cp is the specific heat capacity of the fluid.

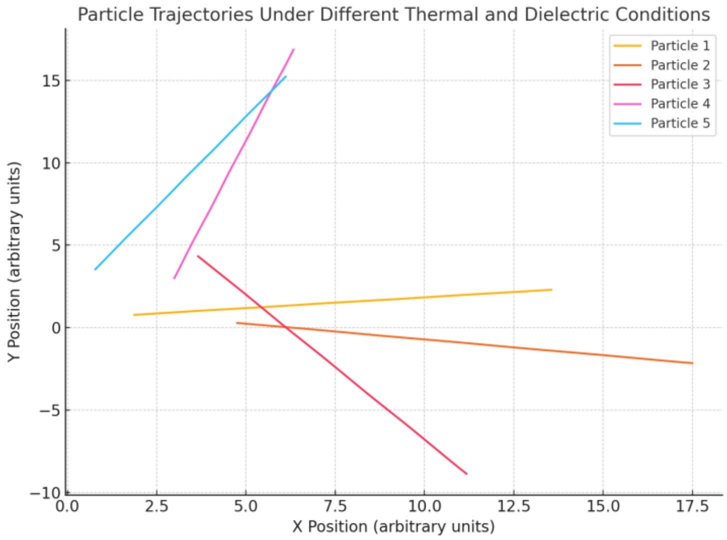

Figure 2. Particle Trajectories under Different Thermal and Dielectric Conditions

Figure 2 shows how colloidal particles move due to the influence of different thermal and dielectric situations. The trajectories of the motion of other particles are displayed as different lines, and the variation of the paths indicates how temperature gradients and electric field variations affect the particle. The trajectories experience small variations in both the direction and speed as they move through the system, simulating the applied Joule heating and dielectrophoresis on the particles as specific reactions to their positions. This figure is used to comprehend the interaction between thermal actions and dielectric grading to influence the particle response in micro fluidic gears.

Impact of Joule Heating

Joule heating causes the temperature of the fluid to be distributed unevenly and this affects the viscosity of the fluid and the development of the electrophoretic mobility of the particles directly. The viscosity alteration plays the main role since it determines the stream of the fluids, and the speed of particles [18]. Because of Joule heating, a decrease in viscosity becomes possible and the mobility of the particles becomes higher which is described as:

$$v = \mu(T)E$$

Where:

a. μ (T) is the temperature-dependent mobility.

b. E is the applied electric field.

The Table 2 shows variations in Particle Velocity with increasing Joule heating and Temperature effects.

Table 2. Difference in the Velocity of Particle with Enhancing Joule Heating and Temperature Effects

Joule Heating (W/m³)	Particle Velocity (m/s)	Fluid Viscosity (Pa·s)	Temperature (°C)
1×1031 \times 10^31×103	0.05	0.0018	20
5×1035 \times 10^35×103	0.12	0.0012	35
1×1041 \times 10^41×104	0.18	0.0009	50
2×1042 \times 10^42×104	0.22	0.0006	65

The viscosity η is inversely proportional to temperature T, as shown in the relation:
Where:

$$\eta(T) = \eta 0 e^{A}_{T}$$

a. η0 is the initial viscosity at temperature T0,

b. A is a constant that depends on the fluid type.

This change in viscosity as a function of temperature impacts the electrophoretic velocity as discussed earlier [19].

Impact of Dielectric Gradient

Particle mobility is altered by the dielectric gradient based on the strength of the electric field generated so that the field strength varies across the medium. In case of a nonuniform dielectric constant ϵ of the medium, the electric field $E^{\rightarrow}$ does not have any homogeneity and this changes the influence of forces on the particles [20].

$$F_{\mathrm{DEP}} = \frac{2\pi r^3 \in 0 \in_m}{3} \nabla E^2$$

The particle is subjected to a dielectrophoretic force which is proportional to the gradient of the dielectric constant:

Where:

a. FDEP is the dielectrophoretic force,
b. r is the radius of the particle,
c. ϵ0 is the permittivity of free space,
d. ϵm is the dielectric constant of the medium, and
e. ∇E2 is the gradient of the square of the electric field.

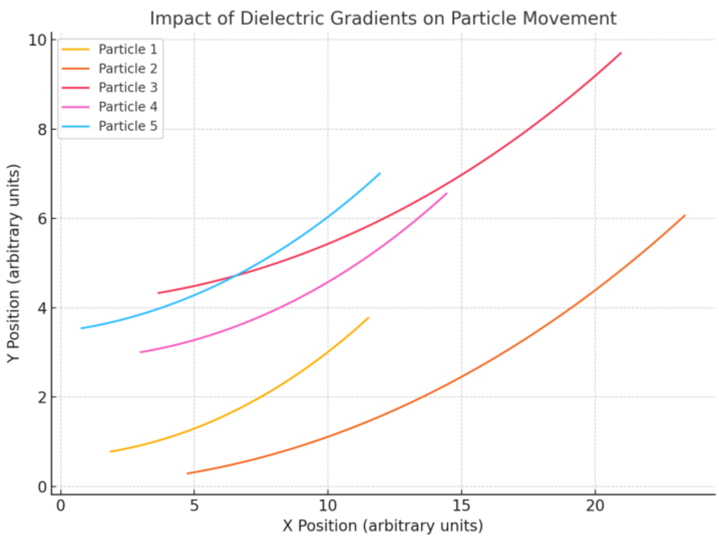

Figure 3. Influence of Dielectric Gradients on the Movement of Particles

Figure 3 indicates how different dielectric gradients within a system influence movements of particles. Non-equal dielectric constants in various regions results in particles having differing trajectories because different places exert different electrostatic forces on these particles. Such an effect may be exploited in microfluidic devices as a sorting or trapping effect.

Coupled Effects

A more important discovery in the simulation is the combination effect of Joule heating and dielectric gradient. The non-linear coupling effect involving thermal effects and dielectrophoresis is quite important resulting in altered behavior of the particles especially at the stronger electric strength of the field. Viscosity of the fluid also lowers because of the temperature gradient created through Joule heating which causes particles to move freely. The dielectric gradient however, also changes the electrostatic forces that arise on the particles and this gives rise to the complex particle trajectories. The combined action of the two phenomena is the strongest when the electric field strength is high since, the dielectrophoretic forces are then more intense in regions where the electric dielectric contrast is high.

The interaction of Joule heating and dielectric gradient may be expressed in terms of the following generalized equation of force encompassing not only the Joule heating but also dielectrophoresis effects:

$$F_{total} = F_{electrostatic} + F_{thermal} = \frac{2\pi r^3 \in 0 \in_m}{3} \nabla E^2 + \mu(T)E$$

Where:

a. Ftotal is the total force acting on the particle, which is a sum of the electrostatic and thermal forces.

5. CONCLUSION

Summary of Contributions

The present paper proposes a multi-physics model, which considers the impact of Joule heating and dielectric gradient to colloidal electrophoresis in microfluidic systems. It is the initial combined endeavor to model both of factors together, which gives more real depiction of the behavior of particles in the presence of certain applied electric fields. The model considers temperature and dielectric inhomogeneity and this augments the understanding of the thermal electrokinetic coupling. These results are important to streamline microfluidic instruments and especially biomolecule separation and the control of nanoparticles.

Research Contributions

The primary innovation is the creation of unified computational model that has both the effects of thermal (through Joule heating) and dielectric gradient. The method increases prediction of particle mobility and separation efficiency. With experimental data the model successfully links fluid dynamics, electrostatics and thermal effects and as such is invaluable in the development of lab-on-a-chip devices.

Future Research Directions

The possibilities of future research may include studying the different behavior of nanoparticles, broadening the model to consider a multi-phase flow, and investigating how this baseline changes when thermal effects combine with particle aggregation. Real time feedback control systems also might integrate to better particle separation and sorting within microfluidic devices making them more adaptable and efficient in microfluidics.

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Author Contributions

Name of Author	C	M	So	Va	Fo	I	R	D	O	E	Vi	Su	P	Fu
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Ravish Kumar	✓	✓	✓	✓	✓	✓	✓		✓	✓	✓	✓	✓	✓

C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

Conflict of Interest Statement
The authors declare no conflict of interest.

Informed Consent
The author's agree to publish the same paper in this Journal.

Ethical Approval
Informed consent and ethical approval sections are included where applicable.

Data Availability
Data available on request from the corresponding author.

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