

Analysis of Transport Phenomena in Water Contaminants with Chemical Reaction in the Presence of Electric Field

R. Sangeetha¹, S. Senthamil Selvi²

¹Research Scholar, Department of Mathematics Vels Institute of Science, Technology & Advanced Studies (VISTAS), Tamil Nadu, India.

²Assistant Professor, Department of Mathematics Vels Institute of Science, Technology & Advanced Studies (VISTAS), Tamil Nadu, India.

Abstract. The transport of water contaminants with chemical reactions in the presence of an electric field is investigated in this article. In this analysis, we look at potential contaminations and their routes. Efforts to remove contaminants from water have resulted in the development of several processes/technologies. The movement of chemically reactive pollutants in a couple stress fluid in the presence of an electric field is described using the generalised dispersion model. For various values of electric number, couple stress parameter, and response rate parameter, analytical findings of dispersion coefficient were obtained. Graphs are used to illustrate the analytical results, and conclusions are drawn. Dispersion rises as the electric number and couple stress parameters rise, but falls when the reaction rate parameter rises.

Keywords: External electric field; Water contaminants, Couple stress fluid, Electric number, Reaction rate parameter.

1. Introduction

Water is found in abundance in both nature and industrial applications. Due to the polar nature of water molecules, an external electric field has a considerable impact on its characteristics [2]. Electric fields are used in a variety of industries, including electrospinning [3&4]. The influence of an electric field on water properties has been investigated through simulations and experiments. Aragonés et al. [2] investigated water phase transitions in an electric field and found that distinct phases of a phase transition occur at different intensities. Contaminations in water disrupt the mechanism's spontaneity, resulting in long- and short-term disorders. Contaminated water is harmful to one's health and can lead to waterborne infections, which can be avoided by taking precautions.

Modeling of water contaminants' movement is the most essential and difficult scientific environmental problem. The molecular diffusion and convection processes are in charge of it. Couple stresses of a larger magnitude have been discovered in fluids. Furthermore, atmospheric ions formed by cosmic rays and natural radioactivity move in the electric field, causing tiny current flows through the atmosphere. The consequence of these water toxins on our environment and human

health is potentially disastrous. Dispersion modelling of water pollutants can be used to forecast this effect. This article's overview is as follows: The introduction of water contaminants and their impacts is covered in Section I. The related work is contained in Section II. Section III & IV describes the methodology for estimating the dispersion coefficient, Section V discusses the experimental results, and Section VI concludes the research work.

2. Related Works

Several researchers have examined dispersion in the presence of a chemical reaction using the generalised dispersion model. Chairatsripatana et al. [7] developed a generalised volumetric dispersion model for a two-phase reaction class. Dulal Pal [8] explored how a chemical reaction affects a solute's dispersion in a porous medium. The global existence of a solution to the Cauchy problem of multidimensional generalised double dispersion equations was studied by Runzhang Xu et al. [6]. High frequency Rayleigh waves in materials with microstructure and couple stress effects were studied by Georgiadis and Velgaki [9]. Mallika and Rudraiah [10] analyzed the influence of the electric field, coupling stress, porous parameter, and slip at the permeable surface on the generalised dispersion of an unstable convective diffusion in a poorly conducting fluid in a channel with porous layers. We can see from the preceding references that using a generalised dispersion model, it is important to examine dispersion on water contaminants with chemical reactions in the presence of an electric field.

3. Methodology

3.1 Ion exchange

Ion exchange is the term used to describe the coulombic attraction between ions and charged functional groups. Ion exchange properties are found in many natural things, including proteins, cellulose, living cells, and soil particles, and they play a crucial role in how they work in nature. Apart from the aforementioned, there is an increasing interest in developing various low-cost adsorbents. Despite the fact that they are called concentration and pressure driven at the same time, both are regulated by the thermodynamic function, or the system's "chemical potential".

3.2 Processes that catalyse

The three most prevalent catalytic processes are nitrate hydrogenation, photocatalytic reactions, and electro catalytic reactions.

3.2.1 Nitrate hydrogenation

Hydrogenation utilising a catalytic process is one of the most promising methods for eliminating nitrate from water. Because the reaction takes place at a low/ambient temperature, very active catalysts are required. The reactions reduce nitrate to the required products, as shown in the reaction scheme, $2 \text{NO}_3^- \rightarrow \text{N}_2 + 2 \text{OH}^-$.

3.2.2 Photo catalytic

The absorption of light with a photo-energy equal to or greater than the semiconductor's band gap triggers photo catalytic reactions in UV-irradiation. To improve catalytic activity using visible light,

analysis of transport phenomena in water contaminants with chemical reaction in the presence of electric field

many ways have been devised, including the incorporation of dopants, the stoichiometry of catalytic metal oxides and mixed metal oxides, particle size and form.

3.2.3 Electro catalytic oxidation

In electro catalysis, the oxidation takes place via a surface mediator on the anodic surface. Temperature, pH, and the diffusion rate of the generating oxidants all influence the rate of oxidation in indirect electrolysis. In contrast to electrolysis, where pollutants are directly oxidised and the rate of oxidation is governed by electrode activity, pollutant diffusion rate, and current density, in electrolysis, pollutants are directly oxidised. Electro catalytic reduction is the most frequent method for eliminating NO₃.

4. Chemical reaction

The main pathways of chemical change of organic molecules in aquatic systems include photolysis, oxidation, hydrolysis, and reduction. In water, photolysis is not an issue. Changes in aquatic systems that affect priority pollutants were gathered and analysed by Callahan (1979). This is simply a brief, high-level overview of chemical processes and their current predictability.

The presence of O₂ is often required for oxidation, but the oxidant is usually free radicals. The concentration of oxidants (e.g., [RO₂⁰],[¹O₂]) and the separate rate constants (e.g., k, RO₂) can be used to indicate the rate of oxidation of an organic compound (OC):

$$-\frac{d[OC]}{dt} = [OC] (k_1[RO_2] + k_2[O_2] + k_3[OH] + \dots) \quad (1)$$

Most organic compounds can have their rate constants predicted using collected, empirical structure-reactivity relationships (Mill, 1980). Reaction rates can be estimated to within a factor of 3-5. The content of free radicals in water, on the other hand, is mostly unknown. Predictions are then restricted to approximations of chemical oxidation rates.

Phenols, aromatic amines, and dienes are among the chemical structures that are most vulnerable to oxidation. Alkenes, halogenated alkenes, alcohols, esters, and ketones are saturated alkyl compounds that may not be significantly oxidizable in water.

Halogens are frequently displaced by hydrolysis (X):



The rate of hydrolysis may also be influenced by surface impacts. When humic material is present, atrazine and other pesticide compounds hydrolyze more quickly. According to Wolfe (1980), such catalytic processes are slow, and structure-reactivity relationships that determine k_H for the hydrolysis rate relationship can be used to provide good estimates of hydrolysis rates at fixed pH:

$$\frac{[]}{[]} = [] \quad (4)$$

An oxidation-reduction reaction is dehalogenation. Although this mechanism is it could be active in low-redox state waters. used to remove a halogen atom in reductive rarely discussed in organic chemical degradation,

According to Esaac and Matsumuna (1980), Eh 0.35 V is needed to make electrons available for dehalogenation. It is a potentially major activity that deserves further investigation because it operates under low-Eh circumstances.

5. Experimental Results

The mathematical modelling of kinetic energy profiles, dispersion coefficient, and mean concentration distribution of water with pair stress is discussed under the influence of a chemical process and an electric field. The data is displayed as graphical representations. In the presence of pair stress, an increase in electric number leads to an increase in kinetic energy. For various values of couple stress, a reaction rate parameter, dimensionless time, and electric number we, the dominating dispersion coefficient values are computed and displayed in figures. The dispersion coefficient increases as the electric number and coupling stress parameter increase.

5.1. The Effect of Water with Chemical Reaction in Electric Field Strength

The process of water condensation on a water with chemical reaction surface is depicted in the diagram below. Clusters will form as the molecules settle on the surface over time. Clusters expand by forming bonds with other clusters and molecules in their vicinity. Due to interfacial tension, water condensing on the surface takes on a spherical shape. The hydrogen atoms change in the water molecules tend to point in one direction when the system is subjected to an electric field strength in one direction, whereas change the oxygen atoms tend to point in the opposite direction in fig 1.

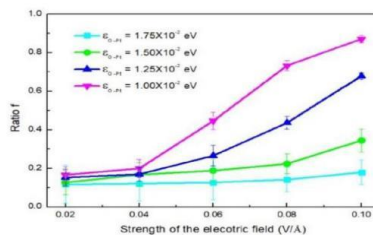


Figure 1. The ratio () varies chemical reaction with the strength of the electric field.

analysis of transport phenomena in water contaminants with chemical reaction in the presence of electric field

The ratio ($\epsilon_{o,h}$), which varies chemical reaction with the strength of the electric field, can affect water condensation on a surface due to polarisation, which reorients the water's molecular dipole moment.

5.2. The Couple Stress of Water with Chemical Reaction in Electric Field

Both water and the electric field force are affected by the condensation of water molecules in an electric field. We looked at how E influences condensation in the previous section. Now we'll look at the interaction between the surface's attraction force and E . When

the potential energy $\epsilon_{o,h}$ is 0.01 eV. In the bulk phase, angle (ϕ) distribution appears to be lower than at the surface. The surface reduces the influence of the electric field on reorientation

by minimising deflection of water molecules at the surface in fig 2.

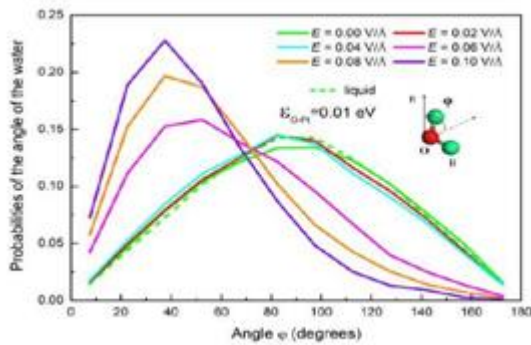


Figure 2. The probability distribution of the angle (ϕ) of the water molecules under different electric fields.

Water causes condensation when there is a chemical reaction difference between the materials in mutual contact. Furthermore, the torsional stress on molecules caused by the electric field. As a result, two criteria can be used to assess the efficiency of energy exchange influenced by the water with chemical reaction in electric field. The first component that influences the efficiency of the water-surface interaction is the amount of water molecules at the surface. The shape of the generated clusters, on the other hand, influences the efficacy of water molecules in fig 3.

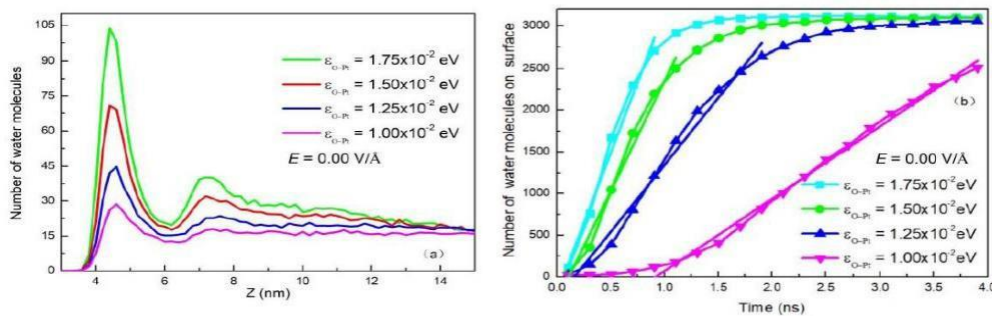


Figure 3. (a) Distribution of water molecules and (b) The number of waters molecules with different chemical reaction in the presence of electric field.

6. Conclusion

In the presence of a chemical reaction, the axial dispersion in a pair stress fluid confined by electrodes at boundaries is investigated using a generalised dispersion model. Water molecule dispersion and mean concentration increase as the electric field and couple stress increase, but when the reaction rate increases, dispersion drops and mean concentration distribution increases. Researchers can use the mathematical model offered here to better understand how reactive air pollutants travel in the presence of an electric field and a pair stress.

Water molecules rotate in the direction of the electric field when an electric field is present, causing a chemical reaction. The reorganisation becomes more obvious as the intensity increases, changing the shape of clusters from spherical to columnar. Furthermore, the density of clusters near the surface decreases as the geometry of the cluster changes. As a result, the condensation rate slows as the electric field intensity increases.

References

1. Pillai, R.; Berry, J.D.; Harvie, D.J.; Davidson, M.R. Electrolytic drops in an electric field: A numerical study of drop deformation and breakup. *Phys. Rev. E*, Vol. 92, 013007, (2015).
2. Aragoes, J.L.; MacDowell, L.G.; Siepmann, J.I.; Vega, C. Phase diagram of water under an applied electric field. *Phys. Rev. Lett.*, Vol. 107, pp. 155701–155704, (2011).
3. Agarwal, S.; Wendorff, J.H.; Greiner, A. Progress in the field of electrospinning for tissue engineering applications. *Adv. Mater.*, Vol. 21, pp. 3343–3351, (2009).
4. Li, D.; Xia, Y. Electrospinning of Nanofibers: Reinventing the Wheel? *Adv. Mater.*, Vol.16, pp. 1151–1171, (2004).
5. Zong, D.; Hu, H.; Duan, Y.; Sun, Y. Viscosity of Water under Electric Field: Anisotropy Induced by Redistribution of Hydrogen Bonds. *J. Phys. Chem. B*, Vol. 120, pp. 4818–4827, (2006).
6. Runzhang Xu, Yacheng Liu and Tau Yu, “Global existence of solution for Cauchy problem of multidimensional generalized double dispersion equations”, *Nonlinear Analysis: Theory, Methods and Applications*, Vol. 71, No.10, pp. 4977-4983, (2009).
7. Chairat Siripatana, Hathaikarn Thongpan and Arwut Promraksa, “Generalised volumetric dispersion model for a class of two phase reaction”. In the proceedings of the 2017 5th International Conference on science & Engineering in Mathematics, Chemistry and Physics, Indonesia. Vol. 820, pp. 1-11, (2017).
8. Dulal Pal, “Effect of chemical reaction on the dispersion of a solute in a Porous medium”, *Journal of Applied Mathematical modeling*, Vol. 23, No.7, pp. 557-566, (1999).
9. H.G. Georgiadis, E.G. Velgaki, “High-frequency Rayleigh waves in materials with micro - structure and couple stress effects”, *International Journal of Solids and Structures*, Vol. 40 No.pp. 2501-2520, (2003).
10. K.S. Mallika and N. Rudraiah, “Generalized dispersion of unsteady convective diffusion in Couple stresses poorly conducting Fluid bounded by Porous layer in the presence of an Electric field”, *World Journal of Engineering*, Vol. 8 No.4, pp. 335-346, (2011).