Electrokinetic-Hydrodynamics: "Bridging the Gap"

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Abstract

A vast majority of engineering problems contain topics related to hydrodynamics and solute transport. Many may also agree that electrostatics can be present in conjunction with hydrodynamics and solute transport in many engineering applications (e.g. electrokinetic soil remediation, gel electrophoresis, *kidney filtration*, etc.). However, there is a disconnect (among the different aspects of the subject) when these concepts are taught to the students in the literature. Although these three topics are simultaneously present in many engineering systems, they are typically taught independently of one another and thus the learners, i.e. the students, are left struggling to connect these concepts by themselves. Electrokinetic-Hydrodynamics (EKHD) is a pedagogical framework that allows for efficient integration of these three topics and their dependence on one another when they are all present in an engineering system. This framework consists of using an "H" format in which two vertical "pillars", i.e. "hydrodynamics" and "solute transport" are bridged by "electrostatics". This bridge, and thus this framework, allows students to make the necessary connections between these three topics which then allows them to effectively tackle engineering problems. Several details of the "H" model will be discussed in this contribution and references to its applications in engineering problems will be made.

Keywords

EKHD, electrostatics, electrokinetics, electro-diffusive convective transport

Introduction

Electrostatics is a phenomenon common to many physical problems in engineering, such as electrophoresis, soil remediation, healthcare applications, etc. The ubiquity of this phenomenon motivates the need for an approach that can facilitate student learning and understanding more effectively. Not only does a student need to understand electrostatic concepts individually, but its coupling with other transport phenomena concepts. Very rarely does electrostatics exist in a system without some other phenomena (i.e. mass transfer, momentum transfer, or energy transfer) occurring simultaneously. However, the presence of an external field complicates even the most basic of transport problems by adding another conservation variable which usually results in the concepts of each conservation principle being taught individually. Electrokinetic-Hydrodynamics (EKHD) presents a pedagogical framework that allows engineering problems with both electrostatic and hydrodynamic concepts to be tackled in a more systematic and efficient pedagogical manner, thus making it easier for the learner to understand and solve the problem.¹ Although the EKHD body of knowledge is very general and applicable to many scientific areas, in this particular paper, we have been motivated by applications related to healthcare engineering including cancer tumor treatment, drug delivery to tumors, and wound healing processes.

Pedagogical Framework

Electrostatics and hydrodynamics are typically introduced in a de-coupled manner, although in reality they very much affect one another. The "H" format presented here is a unified body of knowledge that links these two concepts and allows for a deeper understanding for the learner. EKHD has two central aspects: the motion of fluids under an applied field (i.e.

electrohydrodynamics) and the motion of solutes within the fluids.² As seen in Figure 1, these aspects are represented by the two vertical bars of the letter "H" and are linked by a "bridge" that represents the concepts of electrostatics.



Figure 1. Pedagogical Framework: Power of the "H" Format

With the concepts of electrostatics we can "bridge the gap" between the fluid domain (the continuum domain for fluids in the system) and the solute domain (the discrete domain of particles in the system).

Electrostatic Bridge

First, the understanding of the electrostatics present in the system must be obtained. This can be done by using the conservation of charge equation and applying the proper assumptions. The electrostatic potential, ψ , is a variable within the momentum and species mass conservation equations, so it is ideal to obtain the electrostatic potential profile first.

Gauss's Equation	1	Poisson-Boltzmann (PBE)		Linearized PBE	Inverse Debye Length
$\nabla^2 \psi = \rho_e(\psi)$	Electrical	$\nabla^2 \psi = 2zFc_0 \sinh\left(\frac{zF\psi}{RT}\right)$	Debye-Hückel	$\nabla^2 \psi = \kappa^2 \psi$	$\kappa \equiv \left(\frac{2F^2z^2c}{\varepsilon RT}\right)^{-1/2}$

Figure 2. Electrostatic Approach

Once the electrostatic potential profile is obtained, it can then be implemented into the fluid domain of the system via the electroosmotic velocity term (See Figure 3).

Fluid Domain

The fluid domain is where the first "coupling" occurs. In addition to a hydrodynamic velocity component, the presence of charge presents a new term, the electroosmotic velocity component. Once the proper assumptions are made and the model equation simplified, it can be integrated and the velocity profile obtained.

Navier-Stokes Equation	Electro- Kinetic Force $\vec{f_e} = \rho_e(\psi)\vec{E}$	$\vec{v} = \vec{v_h} + \beta \vec{v_e}(\psi)$ Integrate	Obtain Total Velocity Profile
$\rho\left(\frac{\partial v}{\partial t} + \vec{v} \cdot \vec{\nabla} \vec{v}\right) = -\vec{\nabla}P$	$+\mu\nabla^2\vec{v}+\vec{f_e}(\psi)+\rho\vec{g}$	Total Hydro- Electro- Bulk dynamic osmotic velocity velocity	$\vec{v} = f(x, y, z, \psi)$

Figure 3. Fluid Domain Approach

Solute Domain

Now that the velocity profile has been identified, the next two couplings can occur – the Fluid/Solute coupling and the Solute/Electrostatics coupling. The Fluid/Solute coupling arises via the convective term in the species continuity equation (SCE). In addition, the Solute/Electrostatics coupling is due to the electromigrative flux term in the SCE (See Figure 4).

Species Continuity Equation	Total Molar Flux	-	Simplify,	Obtain Concentration
$\frac{\partial C_A}{\partial t} + \vec{\nabla} \cdot \vec{N_A} = R_A(C_A, T)$	$ \overline{N_{A}} = \underbrace{-D\vec{\nabla}C_{A}}_{\text{Diffusive}} + \underbrace{\vec{v}C_{A}}_{\text{Flux}} + \underbrace{(\mu_{A}C_{A})\vec{\nabla}\psi}_{\text{Flux}} $ Total Diffusive Flux Flux Flux Flux		Integrate Apply BCs	Profile $\overrightarrow{C_A} = f(x, y, z, \psi)$

Figure 4. Solute Domain Approach

Primary Observations and Future Work

The key pedagogical aspect of this contribution is to show all the couplings for a system within EKHD applications. Based on the new framework, a system involving electrostatics, hydrodynamics, and solute transport can be properly analyzed in a systematic way. The couplings allow learners/modelers to understand phenomena native to each domain (such as diffusive transport in the solute domain) and also "hybrid" transport (such as electroosmosis in the fluid domain) that results from the introduction of electrostatics. A course has been taught by using the EKHD framework where students have been exposed to the different aspects of various applications of the subject to separations, colloidal dispersions and their stability and microfluidics. The course used a student-centered and learning approach where teams of students were presented with a challenge and they had to use the framework to develop an understanding of the physics that governs the challenge. Debriefing of the students showed an excellent satisfaction with both the approach and the role played by the framework in the learning process. Future work will include a more systematic and quantitative assessment.

References

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