THESIS

MODELING THE EFFECT OF NONUNIFORM MAGNETIC FIELDS ON IONIC SOLUTIONS

Submitted by
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WE HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER
OUR SUPERVISION BY STEVEN R. BENOIT ENTITLED MODELING THE
EFFECT OF NONUNIFORM MAGNETIC FIELDS ON IONIC SOLUTIONS BE
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OF MASTER OF SCIENCE.

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ABSTRACT OF THESIS

MODELING THE EFFECT OF NONUNIFORM MAGNETIC FIELDS ON IONIC SOLUTIONS

(Pending...)

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CHAPTER 1

Background and Motivation

In an ionic solution, ionic compounds dissociate into their components, which exist independently in solution at some equilibrium concentration. This is possible because the solvent acts to prevent the ions from recombining, as they are naturally inclined to do, given their opposing charges.

The most common ionic solutions are aqueous solutions. An example of such a solution is saltwater, in which sodium chloride dissociates readily. In oceanic seawater or brackish groundwater, additional compounds are dissolved, but most are ionic compounds that dissociate nearly completely in solutions, at the concentrations typically observed.

This, then, provides the primary motivation for examining techniques to manage ions in this type of solution. Desalination of seawater to create potable drinking water or water suitable for irrigation is a high priority for many nations around the world. However, current technologies available in this field are expensive and inefficient, making deployment of commercial-scale desalination plants expensive and limiting their impact on world water supplies. The goal of the present research is to explore an alternative technique that may play a role in a desalination process, potentially at a lower energy cost or reduced complexity than current systems.

1.1. Problem Description

The fundamental problem that needs to be solved is the migration of ions within solution, overcoming natural diffusion effects to create a net concentration gradient. This would allow the separation of the solution into concentrated and dilute regions, which could then become a mechanism for desalination or a subprocess in a larger purification system.

In particular, in a seawater or brackish groundwater solution, sodium chloride, along with many other contaminants, dissociate and become hydrated in solution, forming ion complexes in various concentrations. A hydrated ion consists of a central ion with a number of molecules of solvent clustered around it. This occurs in water because the water molecules are dipolar. Ion complexes form when oppositely charged hydrated ions are attracted and cluster together, but the strength of the attraction is not sufficient to completely displace the hydrating water molecules, so the ions do not recombine. [7]

Current techniques for separation of salt and other contaminants from seawater can be divided into three main categories: Phase-change methods, filtration methods, and electrical methods. Detailed descriptions of these methods are included in the appendix, but a brief description here will serve as an introduction.

Phase-change methods rely on the fact that when water changes state, contaminants tend to remain in the liquid phase. These techniques include distillation, in
1.2. Conceptual Methods

which a sample is boiled or evaporated and the resulting vapor condensed to recover purified water and freezing, in which the contaminants remain in the unfrozen liquid and ice that forms is relatively pure. The advantages of these techniques is that they are simple to understand, and plant construction is relatively simple. However, they are all comparatively inefficient or slow, since the energy required to drive water through a phase change is significant, and all require regular cleaning as scale and residue build up in the vessel where the phase change is taking place.

Filtration methods, which include reverse osmosis, use a membrane and a pressure differential to filter out particulates, large ions, and ion pairs and complexes from the smaller pure water molecules. These systems have the advantage that they will remove not only the salt but other contaminants with complex molecular structure, such as biological agents, and do so at a lower energy cost than phase-change methods. However, they suffer from reliability and maintenance issues as membranes become fouled and break down over time. These systems are also sensitive to the temperature of the water, with higher temperatures shortening the useful life of the membranes.

The only electrical method currently in use is a form of dialysis in which a current is passed through the sample as it flows through an alternating series of filtration membranes. The current causes the ions in the solution to act as charge carriers, with cations flowing one direction and anions flowing the opposite direction. The membranes alternate between those that pass cations and those that pass anions, leaving purified water in certain channels and concentrated water in the others. While this technique is relatively efficient, and does not require extreme temperatures, it requires a complicated system of alternating membranes which require regular maintenance.

1.2. Conceptual Methods

1.2.1. Electrostatic Approach. Because the problem revolves around removal of charged entities from a solution, it is natural to think about using the inherent charge to migrate ions and to affect localized concentration levels in the solution.

A naïve first approach to is to apply an electric field to a sample, and attempt to migrate cations toward the negative electrode, and anions toward the positive electrode. A quick calculation shows this to be entirely impossible, however, based on the size of Avogadro’s number relative to the electron charge densities that can be achieved on an electrode.

Consider such an experiment:

Assume a 1 ml sample of water, containing a typical concentration of salt found in seawater, or approximately 19 g/kg of chloride and 10.5 g/kg of sodium is between two (infinite for simplicity) conducting plates 1 cm apart.

Given the atomic weights of sodium and chloride, we can obtain the mole fractions of these two ions in solution as follows:

\[ n_{Na} = \frac{0.0105 \text{ g}}{23.00 \text{ g/mol}} = 4.55 \times 10^{-4} \text{ mol} \]

\[ n_{Cl} = \frac{0.019 \text{ g}}{35.45 \text{ g/mol}} = 5.36 \times 10^{-4} \text{ mol} \]
Note that the concentration of chloride ions is higher than that of the sodium ions due to contributions from other contaminants such as magnesium chloride, calcium chloride and potassium chloride, but for this thumbnail estimate we will ignore the associated cations.

Then we can estimate, say, the number of anions in the solution using Avogadro’s number, by

\[ n_{\text{anion}} = (5.36 \times 10^{-4} \text{ mol})(6.02 \times 10^{23}/\text{mol}) = 3.23 \times 10^{20} \]

To electrostatically remove these anions from the solution, we would have to place an insulator between the electrodes and the sample (to prevent conduction through the sample, which would not change ion distributions) and have a number of charges on each plate equal to the number of ions to be migrated to the edges of the sample. The charge density required is given by

\[ \rho = (3.23 \times 10^{20} \text{ ions})(1.6 \times 10^{-19} \text{ C/ion})/\text{cm}^2 = 51.7 \text{ C/cm}^2 \]

Treating the system as a parallel-plate capacitor, and using a dielectric constant of 80 for seawater [19], we can derive the capacitance by [12]

\[ C = 80 \times \frac{1 \text{ cm}^2}{4\pi \cdot 1 \text{ cm}^2} \times \frac{1 \text{ F}}{9 \times 10^{11} \text{ cm}} = 7.07 \times 10^{-12} \text{ F} \]

Then the potential difference required to separate the ions from solution is given by

\[ \Phi = \frac{Q}{C} = \frac{51.7 \text{ C}}{7.07 \times 10^{-12} \text{ F}} = 7.31 \times 10^{12} \text{ V} \]

If voltages in this range were achievable at all, any insulator that was placed between the plates and the sample would break down and conduct long before the required charge density was reached.

Attempts to overcome this problem, by shrinking the sample thickness to reduce ion counts, or employing insulators of extremely high breakdown voltage still cannot overcome the shear magnitude of the required charge density, and result in increasing cost and complexity. Perhaps as nanotechnology advances, scales can be achieved that are small enough to use an electrostatic approach, but it is infeasible today.

1.2.2. Magnetostatic Approach. Given the futility of an electrostatic approach, we look to other ways of using the charge of the ions to control their location. Upon reflection, this is similar to the problem faced by nuclear fusion engineers working to confine plasma to a reaction chamber without contact with physical walls. The fusion problem is that of containing materials in the 100 million degree temperature range, so the task is very difficult given the average kinetic energy of the particles. However, the basic approach, which uses nonuniform magnetic fields, termed a “magnetic bottle”, to contain the charged plasma ions, should be applicable to collections of ions in other settings as well.

The phenomenon this technique relies on is that any charged particle traveling in a magnetic field will experience an acceleration perpendicular to both the velocity of the particle and to the applied magnetic field. A uniform field induces a helical trajectory for a free particle. In a nonuniform field, however, a particle moving in the direction of changing magnetic field density will have a generally helical...
trajectory, which will shrink and slow over time, eventually reversing direction and moving back toward a region of lower magnetic field density. [12]

What must be determined is the strength of this effect relative to that of other processes such as diffusion in the sample, and the resulting steady-state ion distribution as a function of space under a particular magnetic field configuration. This determination forms the basis of the present research.
Chapter 2

Ionic Solutions

The modeling of ionic solutions is a complex and multidisciplinary challenge, depending on the intended usage of the model. For the present research, we will focus on their inorganic chemical, thermodynamic, physical, and electromagnetic properties.

2.1. Aqueous Solutions

The most common ionic solutions encountered are aqueous solutions, with water acting as the solvent. These solutions are also called electrolytic, since they conduct electricity, with their free ions acting as charge carriers. In particular, seawater can be considered a multicomponent electrolytic solution of a number of salts, with other impurities – organic and inorganic – present in smaller quantities. Water, as the solvent and principal component, deserves some attention as its unique properties determine the gross behavior of any aqueous solution.

2.1.1. Water. Pure water, with an ionization constant \( K_w \) of \( 1.00 \times 10^{-14} \), consists of \( \text{H}_2\text{O} \) molecules in equilibrium with \( \text{H}^+ \) and \( \text{OH}^- \) ions, each with a concentration of \( 1.00 \times 10^{-7} \text{ M} \). \( \text{H}_2\text{O} \) molecules consist of two hydrogen atoms bound to a single oxygen atom, with an angle between the two O-H bonds of approximately 105° as shown in Figure 2.1.1.

![Figure 2.1.1. The Water Molecule](image)

The Van Der Waals radius of Hydrogen is 1.20 Å, that of Oxygen is 1.40 Å, and the O-H bond length is 0.95 Å. The asymmetric nature of the water molecule results in an electric dipole moment \( p \) of \( 6.2 \times 10^{-30} \text{ C} \cdot \text{m} \), and it is this charge differential that makes water molecules cluster around free ions, preventing them from recombining, and is what makes water act as such an effective solvent.
2.1. AQUEOUS SOLUTIONS

When water is in the frozen state, molecules align in a crystalline structure. Upon melting into the liquid state, the molecules break that structure and actually pack more tightly, increasing density until 4° C, when density again begins to increase with temperature, as thermal collisions disorder the molecular arrangement. However, in liquid water at the temperatures we are considering, some organization remains, although its structure is not entirely understood. Observations support either tetragonal structures, or a pentagonal dodecahedral structures, but with no patterned repetition or orientation. Some basic properties of water are given in Table 2.1.1. [11]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific Heat (20°C)</td>
<td>$4.18 \times 10^3$ J/kg °C</td>
</tr>
<tr>
<td>Latent Heat of Fusion</td>
<td>$3.33 \times 10^5$ J/kg</td>
</tr>
<tr>
<td>Latent Heat of Vaporization</td>
<td>$2.26 \times 10^6$ J/kg</td>
</tr>
<tr>
<td>Dielectric Constant, (20°C)</td>
<td>80.20</td>
</tr>
<tr>
<td>Density (20°C)</td>
<td>0.9982 g/cm³</td>
</tr>
</tbody>
</table>

Table 2.1.1. Properties of pure water

2.1.2. General Effects of Ions in Solution. Ions, when present in solution, tend to inhibit the formation of ordered arrangements of the molecules, which has the effect of lowering the freezing point, and lowering the temperature where the maximum density is reached. In fact, in seawater, the concentration of ions is high enough that its density decreases as it is cooled all the way to the freezing point.

2.1.3. Seawater. An “artificial seawater” solution, that closely simulates actual seawater in its composition and behavior can be created by combining the materials listed in Table 2.1.2.

<table>
<thead>
<tr>
<th>Material</th>
<th>Mass (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
<td>965.551</td>
</tr>
<tr>
<td>NaCl</td>
<td>23.497</td>
</tr>
<tr>
<td>MgCl₂</td>
<td>4.981</td>
</tr>
<tr>
<td>Na₂SO₄</td>
<td>3.917</td>
</tr>
<tr>
<td>CaCl₂</td>
<td>1.102</td>
</tr>
<tr>
<td>KCl</td>
<td>0.664</td>
</tr>
<tr>
<td>NaHCO₃</td>
<td>0.192</td>
</tr>
<tr>
<td>KBr</td>
<td>0.096</td>
</tr>
</tbody>
</table>

Table 2.1.2. 1 kg of artificial seawater

When seawater is analyzed, it is found to contain concentrations of ions given in Table 2.1.3. The total salinity, or the sum of all cation and anion concentrations, is 34.482 g/kg.
2.1.4. Requirements for Usable Water. According to guidelines published by the United States Environmental Protection Agency (EPA), water used for irrigation should have a maximum salinity of approximately 0.5 g/kg, or up to 1.0 g/kg if the water is to be used on salt-tolerant crops. These figures correspond to removal of approximately 98.5% or 97% of the total dissolved solids (TDS) from seawater, respectively.

If desalinated seawater is used as a supply of potable water, it must meet EPA requirements for maximum levels of all contaminants, which stipulate TDS no greater than 0.5 g/kg, chloride levels no greater than 0.25 g/kg, and sulfate levels no greater than 0.25 g/kg.

Moreover, the concentration of borates in the resulting water must be below 0.75 mg/kg [4] to prevent damage to crops and soils if the water is to be used for irrigation.

<table>
<thead>
<tr>
<th>Ion</th>
<th>Concentration</th>
<th>Molarity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chloride (Cl(^-))</td>
<td>18.980 g/kg</td>
<td>0.535 Molar</td>
</tr>
<tr>
<td>Sodium (Na(^+))</td>
<td>10.556 g/kg</td>
<td>0.459 Molar</td>
</tr>
<tr>
<td>Sulfate (SO(_4^{2-}))</td>
<td>2.649 g/kg</td>
<td>0.028 Molar</td>
</tr>
<tr>
<td>Magnesium (Mg(^{2+}))</td>
<td>1.272 g/kg</td>
<td>0.052 Molar</td>
</tr>
<tr>
<td>Calcium (Ca(^{2+}))</td>
<td>0.400 g/kg</td>
<td>0.010 Molar</td>
</tr>
<tr>
<td>Potassium (K(^+))</td>
<td>0.380 g/kg</td>
<td>0.010 Molar</td>
</tr>
<tr>
<td>Bromide (Br(^-))</td>
<td>0.065 g/kg</td>
<td>0.0008 Molar</td>
</tr>
<tr>
<td>Borate (H(_2)BO(_3^-))</td>
<td>0.026 g/kg</td>
<td>0.0004 Molar</td>
</tr>
<tr>
<td>Strontium (Sr(^{2+}))</td>
<td>0.013 g/kg</td>
<td>0.00015 Molar</td>
</tr>
<tr>
<td>Fluoride (F(^-))</td>
<td>0.001 g/kg</td>
<td>0.00005 Molar</td>
</tr>
</tbody>
</table>

Table 2.1.3. Ion concentrations in seawater
CHAPTER 3

Mathematical Models

In creating the mathematical models for this system, we will first focus on the steady-state behavior of the system, assuming a pseudostatic system which exists in equilibrium. Once this analysis is complete, we move on to estimate the rate at which the system will come to equilibrium, and from that estimate potential rates of treatment.

3.1. Basis of the Model

The system to be modelled consists of a container of untreated water with some concentration of ionic solutes. An arrangement of conductors will be placed around or through the container, insulated from the solution, through which a current will be passed. The configuration that embodies a particular steady-state “experiment” will consist of a description of the shape of the container, the initial concentration of the solution, and the arrangement of current-carrying conductors relative to the container. The model will then predict the steady-state ion concentration distribution.

In the dynamic analysis we add source and sink points in the container, where new untreated solution is introduced, and both the treated solution and a concentrated waste product are removed. A particular experiment will consist of specifying initial ion concentrations in the initial solution and in the solution introduced at the source points, and the position and flow rate of each source and sink point. The model will then predict the ionic concentrations at the sink points.

3.2. Model of the Magnetic Field

We will assume that the magnetic field will be generated by current loops that can be specified as part of the experimental setup. To generalize this to systems that include permanent magnets will be a simple matter of modeling those magnets as fixed arrangements of current loops.

Because we begin by assuming steady-state ion concentrations in a sample, we will disregard any contributions to the magnetic field by migrations of ions within the sample. This will not be true as the solution is coming to equilibrium, and will have to be considered in the study of the system’s dynamic behavior.

Generation of the model of the magnetic field is simplified by the fact that the magnetic permeability of water is almost identical to that of air [11]. If we assume that the experimental apparatus is surrounded by air, as opposed to a material of very different permeability such as iron, then it is not necessary to model the deformation of the field due to regions of differing permeability. Given this, the
magnetic field is given by the Biot-Savart law \([12]\):

\[
\vec{B}(\vec{x}) = \frac{\mu_0 I}{4\pi} \left( d\vec{\omega} \times \frac{\vec{x} - \vec{\omega}}{|\vec{x} - \vec{\omega}|^3} \right)
\]

The domain of the integral in this equation consists of all current elements contributing to the field, where \(\vec{B}(\vec{x})\) is the magnetic field \(\vec{B}\) at a point \(\vec{x}\), \(\mu_0\) is the permittivity of free space, \(I\) is the current carried by an element, \(d\vec{\omega}\) is a differential current element, taken in the direction of positive current flow, and \(\vec{\omega}\) is the position of the differential current element.

Once the magnetic field \(\vec{B}(\vec{x})\) is determined, the equation for the Lorentz force exerted on a charged particle by its motion through that field is given by \([12]\):

\[
\frac{d\vec{v}}{dt} = \frac{q}{m} \sqrt{1 - \frac{v^2}{c^2}} \vec{v} \times \vec{B}
\]

where \(\vec{v}, v, q\) and \(m\) are the particle’s velocity, speed, charge and mass, respectively.

Consider a magnetic field \(\vec{B}\) generated by two distinct current elements. By the linearity of the integral in the Biot-Savart law, the resultant magnetic field is the sum of the contributing fields, \(\vec{B}_1\) and \(\vec{B}_2\). It then follows that the resultant Lorentz force is the sum of the forces due to each component field, since

\[
\frac{d\vec{v}}{dt} = \frac{q}{m} \sqrt{1 - \frac{v^2}{c^2}} \vec{v} \times (\vec{B}_1 + \vec{B}_2)
\]

This implies that we can consider the net force on a particle due to a simple differential current element, then integrate that force expression over all current elements in the system to obtain the total force on the particle.

This represents a substantial simplification in the analysis of the system, since we can begin by disregarding details of a particular arrangement of currents about the apparatus and examine the effect of a single current element. This fact also suggests that caution must be used in the analysis of the effects of the field on particles. Since we can consider the effect of a single current element, then any net force we expect to find must be a sum of the individual forces generated by each current element. This implies that this force will come from the curvature of the magnetic field produced by a small current element, since a purely symmetric field would simply result in the particle orbiting in a helical path. Therefore, during the analysis of the effects of this magnetic field, any linearization of the equations to assume the magnetic field is a constant must be stringently avoided.

### 3.3. Model of Solution Thermodynamics

The determination of average net force on a collection of ions in solution is based on the motion of those ions and requires some knowledge of the speed of the ions. Thermodynamics gives an expression for the distribution of particle speeds in an ideal gas based on its internal energy (temperature). What we would like to have is an expression for the number of particles that have a speed between some value \(v\) and \(v + dv\), relative to the total population of particles. Then we can integrate over this expression to obtain the entire population.
Clearly, the velocity distribution in a liquid will differ from that in a gas, since the nature of molecular interactions are different. But, the concepts of equipartition of energy and the fact that temperature is a measure of internal kinetic energy, divided among the available degrees of freedom in a substance are still valid, so we can expect that the distribution will be similar to that in gases.

### 3.3.1. Maxwell-Boltzmann Speed Distribution

An expression for the distribution of molecular speeds in ideal gases was derived by Maxwell in 1859. Boltzmann later refined Maxwell’s work, and the result is known as the Maxwell-Boltzmann distribution.

A formulation of the Maxwell-Boltzmann speed distribution that gives the number of particles with a certain speed, is given by:

\[
\frac{dN_v}{N} = \frac{4}{\sqrt{\pi}} \beta^3 v^2 e^{-\beta^2 v^2} dv
\]

where \(dN_v\) is the number of particles with velocity between \(v\) and \(v + dv\), \(N\) is the total number of particles in the system, and the constant \(\beta\) is determined by the internal energy of the material [15].

### 3.3.2. Estimation of \(\beta\)

To achieve any quantitative results for resultant forces, we will require a numeric value of \(\beta\). From thermodynamics, we know that at a given temperature, the kinetic energy of the component particles in any particular degree of freedom is \(\frac{1}{2}kT\) [15], where \(k\) is the Boltzmann constant and \(T\) is the temperature in Kelvin.

For a material at 20°C with three translational degrees of freedom, this gives an average translational kinetic energy of

\[
E = \frac{3(1.38 \times 10^{-23} \text{ J/K})(293.15 \text{ K})}{2} = 6.07 \times 10^{-21} \text{ J}
\]

Even though the ions in solution we are interested in are typically embedded in hydrated complexes, the ions remain dissociated and hence have no other modes of vibration, so this estimate of speed should be reasonably valid.

Water molecules have mass 0.018 kg/mol, or 2.99 \times 10^{-26} \text{ kg per molecule}, and the RMS speed of a molecule is related to its translational energy by \(E = \frac{1}{2}mv^2\), or \(v^2 = \frac{2E}{m}\). From the values above, we arrive at an RMS velocity for water molecules of 637 m/s.

Then from the Maxwell-Boltzmann distribution, the RMS speed is related to the value of \(\beta\) by [15]:

\[
\beta = \sqrt{\frac{3}{2}} \frac{1}{v_{rms}}
\]

Using our estimated RMS speed, we find that \(\beta\) is approximately 1.92 \times 10^{-3} \text{ s/m}, giving the speed distribution shown in Figure 3.3.1.

Carrying out the same computations for the other constituents of seawater gives values of \(\beta\) and RMS speeds for those ions, as shown in Table 3.3.1.

### 3.4. Simplifications of the Mathematical Models

In this section, we reexamine the mathematical model developed here, and apply any simplifications we can, without compromising the integrity of the model with respect to the phenomena we are studying.
3.4. SIMPLIFICATIONS OF THE MATHEMATICAL MODELS

![Figure 3.3.1. The Maxwell-Boltzmann Distribution for Water](image)

**Table 3.3.1. β Values by Ion Species**

<table>
<thead>
<tr>
<th>Ion/molecule</th>
<th>Mass (kg)</th>
<th>RMS speed (m/s)</th>
<th>β (s/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water (H$_2$O)</td>
<td>$2.99 \times 10^{-26}$</td>
<td>637</td>
<td>$1.92 \times 10^{-3}$</td>
</tr>
<tr>
<td>Chloride (Cl$^-$)</td>
<td>$5.88 \times 10^{-26}$</td>
<td>454</td>
<td>$2.70 \times 10^{-3}$</td>
</tr>
<tr>
<td>Sodium (Na$^+$)</td>
<td>$3.82 \times 10^{-26}$</td>
<td>565</td>
<td>$2.17 \times 10^{-3}$</td>
</tr>
<tr>
<td>Sulfate (SO$_4^{2-}$)</td>
<td>$1.59 \times 10^{-25}$</td>
<td>276</td>
<td>$4.44 \times 10^{-3}$</td>
</tr>
<tr>
<td>Magnesium (Mg$^{2+}$)</td>
<td>$4.03 \times 10^{-26}$</td>
<td>549</td>
<td>$2.23 \times 10^{-3}$</td>
</tr>
<tr>
<td>Calcium (Ca$^{2+}$)</td>
<td>$6.65 \times 10^{-26}$</td>
<td>427</td>
<td>$2.87 \times 10^{-3}$</td>
</tr>
<tr>
<td>Potassium (K$^+$)</td>
<td>$6.49 \times 10^{-26}$</td>
<td>433</td>
<td>$2.83 \times 10^{-3}$</td>
</tr>
<tr>
<td>Bromide (Br$^-$)</td>
<td>$1.32 \times 10^{-25}$</td>
<td>303</td>
<td>$4.05 \times 10^{-3}$</td>
</tr>
<tr>
<td>Borate (H$_2$BO$_4^-$)</td>
<td>$9.93 \times 10^{-26}$</td>
<td>350</td>
<td>$3.50 \times 10^{-3}$</td>
</tr>
<tr>
<td>Strontium (Sr$^{2+}$)</td>
<td>$1.45 \times 10^{-25}$</td>
<td>289</td>
<td>$4.24 \times 10^{-3}$</td>
</tr>
<tr>
<td>Fluoride (F$^-$)</td>
<td>$3.15 \times 10^{-26}$</td>
<td>621</td>
<td>$1.97 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

### 3.4.1. The Biot-Savart Law

Since we have shown that we may analyze a single differential current element at a time, we can form an expression for the differential magnetic field element, deferring integration until we have a force expression.

\[
d\vec{B}(\vec{x}) = \frac{\mu_0 I}{4\pi} \left( d\vec{\omega} \times \frac{\vec{x} - \vec{\omega}}{|\vec{x} - \vec{\omega}|^3} \right)
\]

### 3.4.2. The Lorentz Force Law

Based on the distribution of particle speeds given by the Maxwell-Boltzmann distribution, it is clear that the relativistic correction term in the force equation can be neglected, leaving

\[
\frac{d\vec{v}}{dt} = \frac{q}{m} (\vec{v} \times d\vec{B})
\]
CHAPTER 4

Steady-State Analysis

In this chapter, we determine the force experienced by a charged particle undergoing thermal motion in the presence of a magnetic field generated by a differential current element, and balance that against the diffusion force generated by a concentration gradient to determine a steady-state ion concentration distribution.

We will do this by generating, for any given particle location and initial velocity, a nonlinear model of the magnetic field about the particle based on a Taylor series approximation. From this, we derive a net force equation, and translate this into a potential function that we can then balance against the diffusion potential of our particular solution, generating a steady-state concentration distribution.

4.1. Coordinate System

Suppose we have a particle of charge $q$ and mass $m$ at a point $\vec{P}$, and an element of current $I$ situated at a point $\vec{\omega}$ flowing over differential length $d\vec{\omega}$.

We will work in a standard right-handed Cartesian coordinate system. At first glance, a spherical system centered about the current element seems the better choice, but when we finally integrate about the particle’s location over varying initial velocities, the combination of these two different spherical systems adds significantly to the complexity of the equations.

4.2. Evolution Equations for a Test Particle

We begin by combining the Biot-Savart and Lorentz force equations to generate an expression for the acceleration of a test particle based on its position and velocity, using the differential magnetic field element generated by the current element.

\[
\frac{d\vec{v}}{dt} = \frac{q}{m} (\vec{v} \times d\vec{B}) = \frac{q\mu_0 I}{4\pi m} \left( \vec{u} \times \left( d\vec{\omega} \times \frac{\vec{p} - \vec{\omega}}{|\vec{p} - \vec{\omega}|^3} \right) \right)
\]

Then writing $\vec{v}$ as $\vec{P}'$ and $\frac{d\vec{v}}{dt}$ as $\vec{P}''$ and combining all constant parameters into a single constant $K$ gives the simplified equation:

\[
\vec{P}'' = \frac{K}{|\vec{p} - \vec{\omega}|^3} \vec{P}' \times \left( d\vec{\omega} \times \left( \vec{p} - \vec{\omega} \right) \right)
\]

where $K = \frac{q\mu_0 I}{4\pi m}$
Now, for a particular current element under consideration, the vectors $\vec{\omega}$ and $d\vec{\omega}$ are fixed, and so if we specify the initial conditions $\vec{P}$ and $\vec{P}'$, this expression will, in principle, allow the precise determination of the particles’s trajectory. In practice, however, this results in system of three nonlinear differential equations, which is not easily solved in closed form. Therefore we will estimate the local behavior about the initial conditions using a Taylor series.

4.3. Taylor Series Approximation

The general form of the Taylor series is:

$$\vec{P}(t) = \vec{P}(0) + \vec{P}'(0)t + \frac{1}{2!}\vec{P}''(0)t^2 + ...$$

(4.3.1)

$\vec{P}(0)$ and $\vec{P}'(0)$ are given initial conditions, and $\vec{P}''(0)$ can be computed directly, producing the second-order Taylor series approximation of the function. However, this approximation will result in an estimate that has constant acceleration (namely $\vec{P}''(0)$), hence constant force, which will eliminate the effect we are trying to model. Therefore, we must expand the series beyond this second-order term.

We compute $\vec{P}'''$ by differentiating 4.2.2, yielding the following:

$$\vec{P}''' = \frac{K}{|\vec{P} - \vec{\omega}|^3} \left[ \vec{P}' \times (d\vec{\omega} \times \vec{P}') + \vec{P}' \times \left( d\vec{\omega} \times (\vec{P} - \vec{\omega}) \right) \right]$$

(4.3.2)

$$- \frac{3K}{|\vec{P} - \vec{\omega}|^4} \left[ \vec{P}' \times \left( d\vec{\omega} \times (\vec{P} - \vec{\omega}) \right) \frac{d|\vec{P} - \vec{\omega}|}{dt} \right]$$

Care must be taken in the consideration of the derivative of the norm $|\vec{P} - \vec{\omega}|$.

To perform this computation, we introduce the following lemma.

**Lemma 1.** Given vectors $\vec{A} \in \mathbb{R}^n$ and $\vec{B} \in \mathbb{R}^n$, and using the Euclidean norm,

$$\frac{d|\vec{A} - \vec{B}|}{dt} = \frac{(\vec{A} - \vec{B}) \cdot (\vec{A}' - \vec{B}')}{|\vec{A} - \vec{B}|}$$

**Proof.** Writing out the vector norm

$$|\vec{A} - \vec{B}| = \sqrt{(A_1 - B_1)^2 + ... + (A_n - B_n)^2}$$

Differentiating with respect to time,

$$\frac{d|\vec{A} - \vec{B}|}{dt} = \frac{2(A_1 - B_1)(A'_1 - B'_1) + ... + 2(A_n - B_n)(A'_n - B'_n)}{2\sqrt{(A_1 - B_1)^2 + ... + (A_n - B_n)^2}}$$

$$= \frac{(\vec{A} - \vec{B}) \cdot (\vec{A}' - \vec{B}')}{|\vec{A} - \vec{B}|}$$

□

Using this lemma, and the fact that $\vec{\omega}$ is a constant parameter, 4.3.2 becomes
4.3. TAYLOR SERIES APPROXIMATION

\[ \vec{P}''' = K \frac{1}{|\vec{P} - \vec{\omega}|^3} \left[ \vec{P}' \times (d\vec{\omega} \times \vec{P}) + \vec{P}'' \times (d\vec{\omega} \times (\vec{P} - \vec{\omega})) \right] \]

Finally, we wish to extend the Taylor series one additional term, so we may examine the magnitude of that term’s contribution to the resulting force value to get an idea of the quality of our second-order estimate.

\[ \vec{P}^{(4)} = K \frac{1}{|\vec{P} - \vec{\omega}|^4} \left[ \vec{P} \times (d\vec{\omega} \times \vec{P}) + 2\vec{P}' \times (d\vec{\omega} \times \vec{P}) + \vec{P}'' \times (d\vec{\omega} \times (\vec{P} - \vec{\omega})) \right] \]

Taking \( \vec{P}_0 \) and \( \vec{P}_0' \) to be the initial position and velocity of the test particle, the derivatives of \( \vec{P} \) of orders 2, 3, and 4 at that point gives the terms in the Taylor series.
(4.3.5)
\[ \vec{P}(t) = \vec{P}_0 + t\vec{P}'_0 + \frac{t^2}{2}\vec{P}''_0 + \frac{t^3}{6}\vec{P}'''_0 + \frac{t^4}{24}\vec{P}^{(4)}_0 \]

where:
\[ \vec{P}''_0 = \frac{K}{|\vec{P}_0 - \vec{\omega}|^3} \left( \vec{P}''_0 \times (d\vec{\omega} \times (\vec{P}_0 - \vec{\omega})) \right) \]
\[ \vec{P}'''_0 = \frac{K}{|\vec{P}_0 - \vec{\omega}|^5} \left[ \vec{P}''_0 \times (d\vec{\omega} \times \vec{P}''_0) + \vec{P}''_0 \times \left( d\vec{\omega} \times (\vec{P}_0 - \vec{\omega}) \right) \right] \]
\[ \vec{P}^{(4)}_0 = \frac{K}{|\vec{P}_0 - \vec{\omega}|^7} \left[ \vec{P}''_0 \times (d\vec{\omega} \times \vec{P}'''_0) + 2\vec{P}''_0 \times (d\vec{\omega} \times \vec{P}''_0) + \vec{P}'''_0 \times \left( d\vec{\omega} \times (\vec{P}_0 - \vec{\omega}) \right) \right] \]

4.4. Derivation of the Force Function

The method we use to come up with a net force expression relies on the fact that in thermal equilibrium, particles take on velocities with random orientation having no preferred direction, and speeds obeying some speed distribution, which we have worked out for the Maxwell-Boltzmann case previously.

This distribution of directions and speeds supply a distribution of initial conditions that we can then feed into our Taylor approximation. Given a fixed initial point, we simply integrate the Taylor expression over all possible orientations, and over the weighted distribution of particle speeds. The result is the average particle trajectory from that point. Then taking the gradient of that trajectory gives the force experienced by the average particle, as a function of its position relative to the current element.
Survey of Current Desalination Technologies

This appendix comprises a brief survey of the technologies currently in use for desalination of water. It is by no means intended to be a reference on the topic, but is provided here to give a reader who is unfamiliar with the field a passing understanding so the approach described in this paper can be contrasted to current methods.

There have been several different approaches to removal of salt from water. It is interesting to note that no single technology has proven itself to be the single best solution. There are commercial plants in use today that exploit each of the major techniques described here.

The systems in use can be roughly divided into three categories.

- Phase change methods, in which water is driven through two phase changes (into a gaseous or solid phase, then back to its liquid state)
- Filtration methods, in which the water is driven by pressure through a membrane that selectively passes or blocks molecules and ions.
- Electrical methods, in which an electric current is used to migrate ions.

In each of these methods, we can analyze the energy requirements for desalination as compared to the theoretical minimum energy required by Thermodynamic constraints.

A.1. Distillation

Distillation is the most commonly implemented desalination technique today. The basic concept of distillation is that when saltwater changes phase to a gas, through evaporation or boiling, the salt is not carried into the gaseous phase, being left behind in the vessel where the water was evaporated or boiled. The steam can then be condensed back into purified water in a separate vessel.

Distillation systems typically operate at an energy cost of 6 to 12 kW per 1000 gallons produced.

A.1.1. Distillation by Boiling. One method to distill water is to use a source of heat (from combustion of fossil fuels or electricity), to boil water at normal atmospheric pressure, then cool the steam to condense it into purified water. Using this approach, a large amount of energy must be supplied to vaporize the water, although some of this energy can be recovered through use of the steam to drive turbines, or by using the steam’s heat to drive some other useful process. Because of this, it is not uncommon for this type of plant to be built as a dual-purpose facility, performing power generation as well as desalinating water.

Adding to the raw energy costs of operating these plants is the fact that they require regular maintenance to remove scale fouling, which reduces heat transfer and lowers plant efficiency. To reduce this problem, water can be pretreated with acids
or phosphates, which reduce scale buildup, however adding these chemicals creates a different set of problems to be solved, including corrosion of ferrous materials due to added acids.

A.1.2. Flash Distillation. Flash distillation takes a different approach to driving the water through a phase change. Rather than increasing the temperature, it works by lowering the pressure until the vapor pressure of the water at room temperature exceeds the ambient pressure, and the water vaporizes without added heat. This process, then, requires a partial vacuum be established in a chamber containing saltwater, and the resulting vapor must be pumped into a chamber at normal atmospheric pressure where it condenses back into a liquid.

These systems tend to be more efficient than the heat-based systems, mainly because heat loss and inefficient heat transfer is a primary source of inefficiency for boiling distillers. However, even flash distillation is one of the least efficient techniques for desalination, based on raw energy input for each unit of purified water produced.

A.2. Freezing

Freezing of saline water results in the formation of ice crystals of pure water, which can then be removed from the saline vessel and remelted to obtain fresh water. This technique requires a refrigeration system capable of bringing saltwater to a state where there are ice crystals present, but the water is flowable. Then the ice is separated, and placed in a melting chamber, while the remaining concentrate is discarded. Some variations on this method have been explored, with freezing being done by injecting materials into the water under high pressure that vaporize upon entering the lower pressure environment, removing heat from the water.

A.3. Reverse Osmosis

The reverse osmosis process (sometimes called hyperfiltration), is based on a selectively permeable membrane. Saltwater is passed over one side of this membrane at high pressure, and a small portion of pure water passes through the membrane to the low-pressure side. The remaining concentrate flows over the membrane and is discarded.

Based on the requirement for a high pressure differential, reverse osmosis membranes are constructed in cylinders, with the membrane and a layer of separating material are wrapped many times around a perforated core. High pressure feed water is injected on the outside of the cylinder, with the separating material resisting the pressure, while allowing purified water to flow on the low-pressure side.

The sole source of energy for the process is the maintenance of sufficient pressure in the feed, making it well suited for use aboard ships, although its use in commercial desalination systems is increasing.

The drawbacks of this process are the high cost of membranes, the tendency of the membrane to become fouled over time, and the sensitivity of the membrane to variations in temperature, and to certain contaminants in the feed water that can degrade the membrane's performance.
A.4. Electrodialysis

Electrodialysis is something of a hybrid method, combining electrical migration of ions with selective membranes to achieve separation. In this system the water is placed in a vessel that has an alternating series of selective ion-permeable membranes, and a direct current is subsequently passed through the solution. This causes the ions in solution to migrate as the charge-carriers conducting the current, but the membranes selectively allow only certain types of ions to pass, resulting in a concentration differential at each membrane. The process is shown schematically in Figure A.4.1.

![Electrodialysis Process Diagram](image)

**Figure A.4.1. Electrodialysis Process**

The main problems faced by these systems are that ion concentrations are only affected near the membranes, requiring constant mixing during the process, and the membranes become fouled and require periodic defouling or replacement.
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<tr>
<td>2</td>
<td>James Newton Butler</td>
<td>Ionic equilibrium: A mathematical approach</td>
<td>Addison-Wesley, Reading, Massachusetts</td>
<td>1964</td>
</tr>
<tr>
<td>3</td>
<td>David Eisenberg and Walter Kauzmann</td>
<td>The structure and properties of water</td>
<td>Oxford University Press, New York, New York</td>
<td>1969</td>
</tr>
<tr>
<td>4</td>
<td>Environmental Protection Agency (EPA)</td>
<td>Guidelines for water reuse</td>
<td>US Agency for International Development (USAID), Washington, DC</td>
<td>1992</td>
</tr>
<tr>
<td>6</td>
<td>Kenneth L. Henold and Frank Walmsley</td>
<td>Chemical principles, properties, and reactions</td>
<td>Addison-Wesley, Reading, Massachusetts</td>
<td>1984</td>
</tr>
<tr>
<td>7</td>
<td>H. E. Homig</td>
<td>Seawater and seawater distillation</td>
<td>Vulkan-Verlag, Essen</td>
<td>1978</td>
</tr>
<tr>
<td>9</td>
<td>John P. Hunt</td>
<td>Metal ions in aqueous solution</td>
<td>W. A. Benjamin, Inc., New York, New York</td>
<td>1963</td>
</tr>
<tr>
<td>12</td>
<td>Hans Ohanian</td>
<td>Classical electrodynamics</td>
<td>Allyn and Bacon, Inc., Newton, Massachusetts</td>
<td>1988</td>
</tr>
<tr>
<td>13</td>
<td>S. S. Penner</td>
<td>Thermodynamics for scientists and engineers</td>
<td>Addison-Wesley, Reading, Massachusetts</td>
<td>1968</td>
</tr>
<tr>
<td>15</td>
<td>Francis Weston Sears</td>
<td>An introduction to thermodynamics, the kinetic theory of gases, and statistical mechanics</td>
<td>second ed., Addison-Wesley, Cambridge, Massachusetts</td>
<td>1953</td>
</tr>
<tr>
<td>17</td>
<td>Michael Spivak</td>
<td>Calculus on manifolds</td>
<td>W. A. Benjamin, Inc., New York, New York</td>
<td>1965</td>
</tr>
<tr>
<td>19</td>
<td>John Wright and Angela Colling</td>
<td>Seawater: Its composition, properties and behavior</td>
<td>second ed., The Open University, Milton Keynes</td>
<td>1995</td>
</tr>
</tbody>
</table>