MODEL OF THE SELF-ASSEMBLY PROCESS OF DIELECTRIC NANOSPHERES DEPOSITED BY ELECTROSPRAY

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A i miei genitori,
che, nonostante i tempi bui,
hanno sempre intravisto la luce.

A Luis y a Sandra,
que, con sus paciencia,
me han acompañado en el camino de mi futuro.
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1 Introduction & motivation

In recent years nanotechnology has impacted many research domains and industries to master the nanodimensions to taylor surfaces, materials and properties. In many occasions, nanoparticles and coatings or devices based on them shown interesting new properties or functionalities. In biology, for example, nanoparticles are used in order to build filters that are capable to catch particular bacteria or cells, to make possible a better analysis of the particle selected. So, it is possible, for example, analyze the DNA, in order to detect some blood’s anomalies [1]. Another way to use nanospheres filters is to protect the liquid from some particular bacteria, for example in the case of water’s filter [2][3]. In MEMS ( Micro Electro-Mechanical Systems) as in NEMS (Nano Electro-Mechanical System) often nanoparticles are used technology [4][5]. Recently, nanoparticles technology are also used to fight cancer [6]. The nanospheres are also used in textile field, where it has been discovered that, using polymer’s nanospheres, it is possible to create a new type of tissue hydrofobic, antibacterial, anti odor and stain resistance[7]. The Schoeller industries, for example, use the nanosphere technology in order to create different wear products, in special case it is ideal for use in clothing for such areas as outdoor, sportswear, men’s fashion, women’s wear, career apparel and workwear as well as for shoes and home furnishings.

This technology worked because the nanospheres are regularly organized or self-assembled. In order to make this possible, there are many approaches. We can cite some of them [8]:

1. Drop coating: the attractive capillary force and convective transport of the nanospheres arising from the continuous solvent evaporation are the main factors dominating the self-assembly process, and the ordering and quality of the obtained arrays are largely determined by the evaporation rate.

2. Dip coating: The substrate is immersed in the solution of the coating material at a constant speed. The thin layer deposit itself while it is pulling up. Excess liquid will drain from the surface and then the solvent evaporates from the liquid [9];

3. Spin coating: A small amount of coating material is applied on the center of the substrate. The substrate is then rotated at high speed in order to spread the coating material by centrifugal force [10];

4. Electrophoretic deposition: a thin layer of colloidal suspension is confined between two electrodes, and an applied electric field drives the charged nanospheres to move towards the electrodes, leading to their self-assembly on the electrode interfaces [11].
With those approaches it is also possible to create a new type of mate-
rials, known as **metamaterials**, that, combining nanosphere of differents
materials in a specific geometric position, have properties difficult to find
in nature. One of the most interesting properties discovered is about op-
tics issues [12] [13]. In fact, using specific components and a well defined
nanosphere geometry, it is possible create a material able to have a negative
refraction index, impossible to find in nature. That discovery opened the
world at the **superlenses** that can greatly increase optical resolution beyond
the capability of conventional lenses, becoming a solution to the centuries old
problem of diffraction-limited systems. In other work, a form of **invisibility**
has been demonstrated at least over a narrow wave band. Although the
first metamaterials were electromagnetic, acoustic and seismic metamateri-
als are also areas of active research. Potential application of metamaterials
are diverse and include remote aerospace applications, sensor detection and
infrastructure monitoring, smart solar power management, public safety,
radiomes, high-frequency battlefield communication and lenses for high-gain
antennas, improving ultrasonic sensor, and even shielding structures from
earthquakes. The research in metamaterials is interdisciplinary and involves
such fields as electrical engineering, electromagnetics, solid state physics, mi-
crowave and antennas engineering, optoelectronics, classic optics material
sciences, semiconductor engineering, nanoscience and others.

One of the best techniques used to manipulate nanoparticles is with the
help of an electric field [14]. Recently, several attempts to use dielectrophore-
sis (DEP) as a novel method for nanoparticles manipulation have been made.
This force does not require the particle to be charged, the strength of the
force depends strongly on the medium and particles’ electrical properties,
on the particles’ shape and size, as well as on the frequency of the electric
field. Thus, under the action of spatially non-uniform AC electric fields,
dielectric particles move. DEP methods can be used in many forms (elec-
trorotation, traveling wave DEP, negative and positive DEP) to manipulate
and more generally, to control the position, orientation and velocity of micro-
and nanometric scale particles, including carbon nanotubes and biological
particles such as viruses, DNA, bacteria and cells of various kinds (mass
spectrometer [15]). Since the relative dielectric polarization (and hence the
dielectric response) of the nanoparticles depends on the driving frequency of
the applied electric field, an alternating (AC) electric field is usually applied
to generate DEP forces of different magnitudes and directions.

In order to make possible the nanoparticle manipulation, we must allo-
cate the nanosphere in the middle of the plates. One of the methods most
known to do this is using the **electrospray method** [16] [17]. The way it
works is simple: we use a plane of metal (cathode), for example aluminium,
and a needle (anode), in which one there is a liquid (water or alcohol) full
of nanospheres in suspension, in our case polystyrene nanospheres. If we
apply between the needle and the plane a electric field sufficiently high, it
is formed the **Tailor Cone**, well explained in chapter 3.1, on the tip of the needle, causing so a jet of liquid that, depending of the intensity of the electric field, generate a spray.

In this project we work on an analytical solution for the dielectrophoretic force in an electrospray experiment, creating a model with MATLAB, in order to understand better the behavior of the nanosphere under electrospraying method and dielectrophoretic force (DEP), with special regard for the self-assembly effect.
2 Schwarz-Christoffel mapping and electric field calculation

In this section we describe the calculation of the electric field distribution in a simplified geometry of the electrospray technique consisting in a needle where the nanofluid is injected with the help of a microfluidic pump and a substrate. Figure 1 shows the schematic diagramme of the geometry.

![Schematic diagramme](image1)

Figure 1: Schematic diagramme

For the calculation of the electric field we have considered a simplified geometry as shown in Figure 2

2.1 Fundamental of Schwarz-Christoffel transformation

We have used the Schwartz-Christoffel approximation [18] starting in the Z-plane shown in Figure 2

![Z-plane](image2)

Figure 2: Z-plane

where we have 6 characteristic points: D and E are the edges of the...
needle where the voltage is applied, FA distance is taken half of the real distance needle-ground plane, due to the simmetry of the system, while the points A and B are the edges of the ground plane and C and F are their projections in the DE line. The Z-plane is a complex version of the physical plane rotated $90^\circ$ in such a way that the imaginary axis corresponds to the plane where the needle is located and the real axis corresponds to the distance from the needle (Figure 2).

Before applying the SC transformation to our case, let us review the basics in the general case of a closed polygon as shown in Figure 3.

![Figure 3: Z-plane general case](image_url)

Any point in the Z-plane may be identified by vector. In the example shows in Figure 3, we travel counterclockwise around the closed polygon and, according to the angle definition shown in Figure 3, the distance $(Z - Z_A)$ before and after point A can be written as:

\[
\begin{align*}
\text{before} & \quad Z - Z_A = |Z - Z_A|e^{j\phi_A} \\
\text{after} & \quad Z - Z_A = |Z - Z_A|e^{j(\phi_A - (\pi - \alpha))}
\end{align*}
\]

where $\phi_A$ is the angle between the horizontal axis and the polygon side by the point into consideration and the previous point, in our case, $Z_F$, and $\alpha$ is the angle between the extension of the line constructed by the point into consideration and the previous point and the line constructed by the point into consideration and the following point, $Z_B$ in our case (Figure 3).

Once the Z-plane has been established the SC transformation consists in mapping the points inside the closed polygon into a new T-plane in such a way that all corner points of the Z-plane polygon are mapped onto points in the real axis of the T-plane as shown in Figure 4.
Now the travel around the polygon in the Z-plane is transformed in a travel along the real axis in the T-plane where the distances around one of the points, for example $T_A$, can be written as:

before $T - T_A = |T - T_A|e^{j\pi}$

after $T - T_A = |T - T_A|e^{j0}$

Now, the mapping from Z-plane into T-plane can be written as,

$$Z - Z_A = (T - T_A)^{\frac{1}{p}}$$

and the correspondence of distances is

$$\begin{cases} |Z - Z_A|e^{j\phi_A} = |T - T_A|e^{j\frac{\pi}{p}} \\ |Z - Z_A|e^{j[\phi_A - (\pi - \alpha)]} = |T - T_A|e^{j\frac{\beta}{p}} = |T - T_A| \end{cases}$$

Comparing equations (1):

$$\frac{1}{p} = 1 - \frac{\alpha}{\pi}$$

so the vectors $Z$ and $T$ are related by

$$Z = C T^{1 - \frac{\alpha}{\pi}}$$

$$\frac{dZ}{dT} = C \left(1 - \frac{\alpha}{\pi}\right) T^{1 - \frac{\alpha}{\pi} - 1}$$

$$\frac{dZ}{dT} = C_1 T^{-\frac{\alpha}{\pi}} \quad \text{where} \quad C_1 = C \left(1 - \frac{\alpha}{\pi}\right)$$

In the case of four corners

$$\frac{dZ}{dT} = C_1 |T - T_A|^{-\frac{\alpha}{\pi}} |T - T_B|^{-\frac{\beta}{\pi}} |T - T_C|^{-\gamma} |T - T_F|^{-\delta}$$ (2)
2.2 Schwarz-Christoffel application to the electrospray geometry

Applying Eq.(2) to the electrospray geometry shows in Figure (2) and as the polygon in the Z-plane has all corners rectangular \( \alpha = \beta = \gamma = \delta = \frac{\pi}{2} \) we find that [19]

\[
Z = C_1 \int \frac{dT}{\sqrt{(T - T_A)(T - T_B)(T - T_C)(T - T_F)}} \tag{3}
\]

Equation (3) can be transformed after variable change in an elliptic integral [20]

\[
Z = C_3 F(\omega_1, k_1) + C_2 = C_3 \int_{0}^{\lambda_1} \frac{d\lambda_1}{\sqrt{(1 - \lambda_1^2)(1 - k_1^2\lambda_1^2)}} + C_2 \tag{4}
\]

where

\[
C_3 = \frac{2C_1}{\sqrt{(T_F - T_B)(T_C - T_A)}}
\]

\[
\omega_1 = \arcsin \left[ \sqrt{\frac{(T_C - T_A)(T - T_F)}{(T_F - T_A)(T - T_C)}} \right]
\]

\[
k_1 = \sqrt{\frac{(T_C - T_B)(T_F - T_A)}{(T_F - T_B)(T_C - T_A)}}
\]

\[
\lambda_1 = \sin \omega_1
\]

where \( F(\omega_1, k_1) \) is the elliptical integral of the first kind and \( k_1 \) is the modulus of the elliptic function.

Equation (4) links the T plane to the Z plane. The values of the coefficients \( C_2 \) and \( C_3 \) can be solved by the mapping relationship between the coordinates of the corresponding points in the two planes \( (Z_F \rightarrow T_F, Z_C \rightarrow T_C, Z_B \rightarrow T_B, Z_A \rightarrow T_A) \) leading to,

\[
C_2 = 0
\]

\[
C_3 = \frac{h}{2K(k_1)} = \frac{d_1 + w + d_2}{K(k'_1)}
\]

where \( K(k_1) \) is the complete elliptic integral of the first kind and \( k'_1 = \sqrt{1 - k_1^2} \).

In this manner, it can be written like

\[
\frac{dZ}{dT} = \frac{h}{2K(k_1)} \sqrt{(T_F - T_B)(T_C - T_A)} \left( \frac{1}{2\sqrt{(T - T_A)(T - T_B)(T - T_C)(T - T_F)}} \right) \tag{6}
\]

After the mapping into the T-plane has been completed, a second mapping is performed between the T-plane and a new W plane, in such a way
that the points in real axis in the T-plane are mapped now onto a new closed polygon as shown in Figure 5.
The reason for this transformation is to get a parallel plate geometry where the boundary conditions are the known potential at the two plate and the Dirichlet boundary condition (continuity of potential and electric field) at the two lateral side.

Figure 5: W-plane

The second SCM is used to transform the upper half of the T-plane into a rectangle in the model plane (W-plane). The electric field is uniformly distributed in the interior of the rectangle due to the restriction from the transformed boundaries in the W-plane. The corresponding points are \( W_E = jY_W, \ W_D = X_W + jY_W, \ W_C = X_W \) and \( W_F = 0 \), where \( X_W \) and \( Y_W \) are the size of the rectangle along the real and imaginary axes, respectively. Similarly, the transformation from the T-plane to the W-plane is given by

\[
W = D_1 \int \frac{dT}{\sqrt{(T - T_C)(T - T_D)(T - T_E)(T - T_F)}}
\] (7)

that after variable change also transforms in an elliptic integral

\[
W = D_3 F(\omega_2, k_2) + D_2 = D_3 \int_0^{\lambda_2} \frac{d\lambda_2}{\sqrt{(1 - \lambda_2^2)(1 - k_2^2\lambda_2^2)}} + D_2
\] (8)
with

\[ D_3 = \frac{2D_1}{\sqrt{(T_F - T_D)(T_E - T_C)}} \]
\[ \omega_2 = \arcsin \left( \frac{\sqrt{(T_E - T_C)(T - T_F)}}{(T_F - T_C)(T - T_E)} \right) \]
\[ k_2 = \sqrt{\frac{(T_E - T_D)(T_F - T_C)}{(T_F - T_D)(T_E - T_C)}} \]
\[ \lambda_2 = \sin \omega_2 \]

Equation (8) links \( T \) plane with the \( W \) plane. The values of the coefficients \( D_2 \) and \( D_3 \) can be obtained by a similar mapping procedure to the first SCM performance.

\[ D_2 = 0 \]
\[ D_3 = \frac{Y_W}{K(k'_2)} \]

where \( Y_W \) is the length of the side of the rectangle along the imaginary axis. So, we can write that

\[ \frac{dW}{dT} = \frac{Y_W}{2K(k'_2)} \sqrt{(T_F - T_D)(T_E - T_C)} \]

(10)

Now, to find the electric field in the \( Z \) plane and, as the Laplace equation is conserved in the transformation,

\[ \nabla \phi_Z = \nabla \phi_W f'(Z) = \nabla \phi_W \frac{dW}{dZ} \]

(11)

with

\[ \nabla \phi_W = j \frac{V}{Y_W} \]
\[ \frac{dW}{dZ} = \frac{dW}{dT} \frac{dT}{dZ} \]

so, we find that the electric field is calculated as

\[ E_0 = \nabla \phi_Z = j \frac{2V K(k_1)}{\hbar K(k'_2)} \sqrt{(T_F - T_D)(T_E - T_C)(T - T_A)(T - T_B)(T - T_E)(T - T_D)} \]

(12)

This is the main result of the SC transformation applied in the electro-spray geometry and provides an analytical solution for the electric field at any point inside the original polygon in the physical domain.
The SC transformation has several degrees of freedom and up to three values for the points in the T-plane can be arbitrarily chosen following this criteria [18]:

\[ T_F > T_E > T_D > T_C > T_B > T_A \]

where \( T_A \) is chosen to be equal to 0.

To choose the points \( T_B \) and \( T_C \), we know that \( T_F > 0 \) and hence \( k_1^2 > 1 - \frac{T_B}{T_C} \) where \( k_1 \) is the modulus of the elliptic function. In order to calculate this coefficient, we use the Hilberg’s approximations [21]:

\[
M = \frac{1}{4} e^{\frac{\pi}{4} \left( d_1 + w + d_2 \right)} \quad \text{if} \quad \frac{K(k_1)}{K(k'_1)} \geq 1
\]

\[
M = \frac{1}{4} e^{\frac{2\pi(d_1 + w + d_2)}{h}} \quad \text{otherwise}
\]

where \( K(k_1) \) is the complete elliptic integral of the first kind and \( k'_1 = \sqrt{1 - k_1^2} \). From those equations, we can finally obtain the value of \( T_B \) and \( T_C \). Choosing \( T_B = 1 \), we find \( T_C = 1.0009 \).

From equation (5), we can calculate \( T_F \):

\[
T_F = \frac{T_B(T_C - T_A)k_1^2 - T_A(T_C - T_B)}{(T_C - T_A)k_1^2 - (T_C - T_B)}
\]
To find the other points in the plane $T$, we use the inverse function of Eq.(4)

$$T = \frac{T_FT_Ccn^2\left(\frac{Z}{C_3}, k_1\right)}{T_C - T_Fsn^2\left(\frac{Z}{C_3}, k_1\right)}$$  \hspace{1cm} (14)$$

where $cn$ and $sn$ are the Jacobian elliptic functions and $C_3 = \frac{h}{2K(k_1)}$. With equation (14), we can find the value of $T_D$ and $T_E$.

$$T_D = \frac{T_FT_Ccn^2\left(j\frac{w+d_2}{C_3}, k_1\right)}{T_C - T_Fsn^2\left(j\frac{w+d_2}{C_3}, k_1\right)}$$  \hspace{1cm} (15)$$

$$T_E = \frac{T_FT_Ccn^2\left(j\frac{d_2}{C_3}, k_1\right)}{T_C - T_Fsn^2\left(j\frac{d_2}{C_3}, k_1\right)}$$  \hspace{1cm} (16)$$

Now that we have found all the points in the plane $T$, we can calculate the electric field in the $Z$ plane with Eq.(12).

Figure (7) shows the electric field value at different distances from the needle, for an applied voltage of 10000V, distance between electrodes $h = 10cm$, diameter of the needle $w = 0.3mm$, distance between the needle and the end of the collector plane $d_1 = d_2 = 4.985cm$.

![Figure 7: Absolute Electric Field](image-url)
As we can see in Figure (7), the order of magnitude of the electric field value is in the $10^5 \frac{V}{m}$ range and, more we get closer to the substrate, the electric field becomes smaller. Moreover, we can say that not only becomes smaller, but tends to become constant along the x-axis, but has a gradient along the y-axis, as we can see in Figure (8) and (9).

**Figure 8: Absolute Electric Field on the needle**
The reason why the electric field is not constant near to the needle is because we are not using two plate to induce the electric field, but a plate and a needle.

In order to understand better the behavior of the electric field, let’s change some parameters. For example, if we change the diameter of the needle, the magnitude of the electric field becomes higher and its distribution becomes wider while we increase the diameter dimension (Figure (10)).
Figure 10: Behaviour of the electric field as a function of the needle diameter, $w$

Instead, if we increase the distance between the needle and the ground plate, we found that the magnitude of the electric field decreases (Figure (11)). That means that the distance $h$ is inversely proportional to the electric field, as we can see in equation (12).
Another parameter to take into account is the magnitude of the electric field near the needle. This is shown in figure (12), where it can be seen that the electric field close to the needle edge at the needle is about $3.14 \times 10^6 \text{V/m}$, that means that at the tip of the needle the high value of the field can create a phenomenon called Taylor’s cone [22] as discussed in the following chapter.

Figure 11: Behaviour of the electric field by varying $h$ parameter
Figure 12: Absolute Electric Field near the needle
3 Electrospray process and phases

Our hypothesis of the electrospray deposit process involves three main phases:

1. **Ejection phase of droplets**
2. **Droplet travel towards the substrate**
3. **Landing and drying phase**
3.1 Ejection phase, Taylor cone and droplet charge

When a small volume of electrically conductive liquid is exposed to an electric field, the shape of liquid starts to deform from the shape caused by surface tension alone. As the voltage increases, the electric field exerts a similar amount of force on the droplet as the surface tension does; a cone shape begins to form with convex sides and a rounded tip. This approaches the shape of a cone with a whole angle of \( 98.6^\circ (\theta = 49.3^\circ) [23] \). When a certain threshold voltage has been reached, the slightly rounded tip emits a jet of microdroplets called a conejet and is the beginning of the electrospraying process in which ions may be transferred to the gas phase. It is generally found that in order to achieve a stable conejet a slightly higher than threshold voltage must be used. As the voltage is increased even more, other modes of droplet desintegration are found.

The threshold voltage that sets the Taylor cone, is found from equations [23],

\[
\frac{r_{\text{drop}}}{\pi^2} = \frac{\rho}{4\pi^2 \gamma \tan \left( \frac{\pi}{2} - \theta \right) \left( \frac{U_T}{U_a} \right)^2 - 1}\right) \times \left( \frac{dV}{dt} \right)^{2/3} \tag{17}
\]

\[
U_T = 0.863 \left( \frac{\gamma h}{\varepsilon_0} \right)^{1/2} \tag{18}
\]

\[
q_{\text{drop}} = 8\pi \left( \varepsilon_m \gamma r_{\text{drop}}^3 \right)^{1/2} \tag{19}
\]

\[
F_{\text{drop}} = q_{\text{drop}} |E_0| \tag{20}
\]

where \( r_{\text{drop}} \) is the radius of the water’s drop, that is equal to the radius of the tip of the Taylor’s cone, \( U_T \) is the threshold voltage, \( U_a \) is the applied voltage, \( \gamma \) is the surface tension of the liquid, \( \theta \) is the liquid cone angle (supposed equal to 49.3° for the classical Taylor cone model), \( \rho \) is the density of the liquid, \( \frac{dV}{dt} \) is the flow rate, \( \varepsilon_0 \) is the vacuum permittivity and \( h \) is the distance between needle and substrate.

So, theoretically, if we use water (\( \gamma = 0.073 \)) with a distance \( h = 10\, \text{cm} \) we find that we can reach the Taylor cone if we apply a tension higher than 19kV. However, in the experiment described in [24], it is formed at a lower voltage, typically 8kV. That means that the theoretical value of threshold voltage apparently does not describe accurately the experiment [23].
In figure 13 shows a picture of the Taylor cone when a tension around to 10kV is applied. In fact, we can see that the angle of the Taylor cone is equal to $87^\circ (\theta = 43.5^\circ)$, clearly below that critical angle. When a droplet is created, it has a dimension defined by the $r_{\text{drop}} = 7.57\mu m$ calculated from equation (17). In the experiment registred in [24] spheres of 180nm radius are used and hence we can estimate that in a single droplet can hold more than $3 \times 10^4$ particles.

It is well known that the microdroplets after they are ejected, they start loosing liquid as it evaporates more importantly if there is alcohol involved in the solution and hence the droplets are becoming more and more small. So we can take into account two extreme hypothesis:

1. **The liquid has not yet evaporated totally**: we have a charged drop of liquid, hence subject to Coulomb Force

2. **The liquid is totally evaporated**: we then assume that the nanospheres, which are dielectric, have to be subject to a Dielectrophoretic Force as they are charge-neutral.
Knowing the electric field, we can calculate the forces that this electric field creates on the droplets or particles. On the one side we have the Coulomb force which is simply proportional to the charge and to the electric field value and that is the main component for charged particles, but we also have the Dielectrophoretic force that appears in dielectric spheres polarized under an electric field. This Dielectrophoretic force is proportional to the gradient of the electric field module squared as follows,

\[ F_{\text{DEP}} = 2\pi \varepsilon_m R^3 k \nabla |E|^2 \]  

(21)

where

\[ k = Re\left[ \frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m} \right] \]  

(22)

is the Clausius-Mossoti Factor, where \( \varepsilon_p \) is the polystyrene’s permittivity while \( \varepsilon_m \) is the air’s permittivity.

The Coulomb force’s exerted on the droplets ejected is shown in Figure(14) and that of the Dielectrophoretic force direction on a single particle at several distances from the needle is shown in Figure(15).

![Figure 14: Coulomb’s Force’s direction](image)

![Figure 15: Dielectrophoretic’s Force’s direction](image)
As can be seen the direction of Coulomb force and Dielectrophoretic force are opposite. Moreover Figure(16) shows the modulus of the two forces. Notice that the distance in vertical axes, 0 is near the needle and 0.05 is far from the needle.

![Figure 16: Comparison between two forces](image)

If we compare the Coulomb force with the Dielectrophoretic force, we notice that the Coulomb force is many orders of magnitude stronger than the Dielectrophoretic force. An interpretation of this results is that the Dielectrophoretic force is negligible compared to the Coulomb force and hence in the ejection an travelling phase the droplets are driven towards the substrate by the Coulomb force and that the Dielectrophoretic force, will only be significant if the particles are not inside a droplet because it has dried.
4 Landing and drying phase

4.1 Dielectrophoretic force between two particles

The landing phase is characterized by the deposition of droplets containing nanoparticles on top of the substrate. The observation made in [24] show that several things may happen. On the one hand when the electrically charged droplets fall into the substrate electrode, the electrical charge is collected by the electrode and contributes to the external current in the circuit. Besides, a droplet in the process of drying suffers from the well known effect of "Coffee stain" and the nanoparticles associate randomly due to capillary forces.

However we can make the hypothesis that the nanoparticles are almost free of liquid, beside the interstitial water due to the humidity and can be subject of DEP force.

So we can imagine as a very simple first case, the forces between two dielectric nanoparticles polarized by a constant electric field that are close to each other.

![Figure 17: Electrical dipole](image)

For doing this, it’s better working with polar coordinates $(r, \theta)$, in two dimensions where $r$ is the distance between centers of particles while $\theta$ is the angle between them.

In the geometry considered we have a constant electric field in the $z$-direction and an electric dipole originated by the polarization of the nanoparticle sitting at the origin of coordinates,
4.2 Potential created by a constant electric field

Figure 18: Electrical dipole

Taking into account only the constant electric field, we can calculate the electric potential as,

\[ V = -\int_0^M \vec{E} \, dl \]  

(23)

we can divide this integral in two parts,

\[ V = -\int_0^N \vec{E} \, dl - \int_N^M \vec{E} \, dl \]  

(24)

The first part of the second term is zero because the electric field is orthogonal to the x-axis as it has the direction of Z-axis. So, we find that

\[ V = -E_0 r \cos \theta \]  

(25)
4.3 Potential created by an electrical dipole

![Electrical dipole diagram](image)

Figure 19: Electrical dipole

Taking into account now only the electrical dipole, we can calculate the electric potential at a distance \( r \) from the origin,

\[
V = \frac{q}{4\pi\varepsilon_0 r_1} - \frac{q}{4\pi\varepsilon_0 r_2} = \frac{q}{4\pi\varepsilon_0} \left( \frac{1}{r_1} - \frac{1}{r_2} \right) \quad (26)
\]

Using the triangle equation, we can say that

\[
r_1^2 = r^2 + \left( \frac{d}{2} \right)^2 - rd \cos \theta \quad (27)
\]

\[
r_2^2 = r^2 + \left( \frac{d}{2} \right)^2 + rd \cos \theta \quad (28)
\]

in this manner, we have that

\[
V = \frac{q}{4\pi\varepsilon_0} \left( \frac{1}{\sqrt{r^2 + \left( \frac{d}{2} \right)^2 - rd \cos \theta}} - \frac{1}{\sqrt{r^2 + \left( \frac{d}{2} \right)^2 + rd \cos \theta}} \right) \quad (29)
\]

\[
V = \frac{qd}{4\pi\varepsilon_0} \left( \frac{1}{\sqrt{r^2 + \left( \frac{d}{2} \right)^2 - rd \cos \theta}} - \frac{1}{\sqrt{r^2 + \left( \frac{d}{2} \right)^2 + rd \cos \theta}} \right) \quad (30)
\]

\[
V = \frac{qd}{4\pi\varepsilon_0} f(r, \cos \theta) \quad (31)
\]
4.4 Superposition

Considering now the case when there is a constant electric field with direction in z-axis simultaneously with a dielectric sphere of radius $R$ having its center at the same origin of the coordinates. The potential at a given point $M$ has two components, one originated by electric field $E_0$ and the second originated by the electric dipole due to the polarization of the spherical dielectric particle. We will consider that the total potential has the form of the superposition of the two components described above:

$$V_{\text{out}} = Ar \cos \theta + B f(r, \cos \theta) \quad \text{and} \quad V_{\text{in}} = Cr \cos \theta + D f(r, \cos \theta)$$

where $A$, $B$, $C$ and $D$ are constants that are calculated by means of the application of the boundary conditions. It is required that the potential at $r \to \infty$ should be the potential created by the constant electric field $E_0$ as the other terms vanish. This means that $A = -E_0$. Furthermore, the potential when $r \to 0$ should not tend to infinity, hence $D = 0$

$$V_{\text{out}} = -E_0 r \cos \theta + B f(r, \cos \theta) \quad \text{and} \quad V_{\text{in}} = C r \cos \theta \quad (32)$$

The two additional boundary conditions required to calculate the constants $B$ and $C$ are that the potential inside and outside are the same at the sphere surface as there is no charge (potential is continuous), and that the displacement flux vector $D$ is continuous at the surface. So at $r = R$,

$$V_{\text{out}} = V_{\text{in}} \quad \text{and} \quad \varepsilon_m \frac{\partial V_{\text{out}}}{\partial r} = \varepsilon_p \frac{\partial V_{\text{in}}}{\partial r} \quad (33)$$

where $\varepsilon_m$ is the permittivity of the medium and $\varepsilon_p$ is the permittivity of the particle. Substituting in the equations (33) the equations (32), we find,

$$\begin{cases} -E_0 R \cos \theta + B f(r, \cos \theta) = C R \cos \theta \\ \varepsilon_m[-E_0 \cos \theta + B f'(r, \cos \theta)] = \varepsilon_p C \cos \theta \end{cases} \quad (34)$$

where

$$f' = \frac{\partial f}{\partial r} = -\frac{2r-d \cos \theta}{r^2 + \left(\frac{d}{2}\right)^2 - rd \cos \theta} \quad \text{and} \quad -\frac{2r+d \cos \theta}{r^2 + \left(\frac{d}{2}\right)^2 + rd \cos \theta}$$

Solving the system, we find that

$$\begin{cases} C = \varepsilon_m \frac{E_0 \cos \theta - R E_0 \cos \theta L'}{\varepsilon_m R \cos \theta L' - \varepsilon_p \cos \theta} \\ B = R E_0 \cos \theta \left[\frac{1}{L} + \frac{\cos \theta - R \cos \theta L'}{R \cos \theta L' - f \varepsilon_m \cos \theta} \right] \end{cases} \quad (35)$$

Now, knowing that

$$V_{\text{out-dip}} = B f = \frac{P}{4 \pi \varepsilon_0} f \quad (36)$$
we can calculate an effective dipole $P_{eff}$ as,

$$P_{eff} = 4\pi \varepsilon_0 B = 4\pi \varepsilon_0 R E_0 \cos \theta \left[ \frac{1}{f} + \frac{\cos \theta - R \cos \theta L}{R \cos \theta L - f \frac{\varepsilon_0}{\varepsilon_m} \cos \theta} \right] \quad (37)$$

In this manner, we can say that the electric field is

$$E = -\nabla V = \hat{r} \left[ E_0 \cos \theta - \frac{P_{eff}}{4\pi \varepsilon_0} \frac{\partial f}{\partial r} \right] + \hat{t} \left[ -E_0 \sin \theta - \frac{P_{eff}}{4\pi \varepsilon_0} \frac{\partial f}{\partial t} \right] \quad (38)$$

where

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial \theta} \frac{\partial \theta}{\partial t} = \frac{1}{r} \frac{\partial f}{\partial \theta} = \left[ \frac{\sin \theta}{r^2 + (\frac{d}{r})^2 - r d \cos \theta} - \frac{2 \sqrt{r^2 + (\frac{d}{r})^2 - r d \cos \theta}}{r^2 + (\frac{d}{r})^2 + r d \cos \theta} \right] \quad (39)$$

Figures (20), (21) and (22) show an example of the radial and tangential components of the electric field at a distance $r = 10 \times R$ with $R = 180nm$, and of the module. All three magnitudes are plotted as a function of the angle $\theta$.

![Figure 20: Radial component of Electric field](image)
Figure 21: Tangential component of Electric field

Figure 22: Modulus Electric field
Once the electric field is known we can calculate the force exerted on a second particle located at the distance $r$ from the center at an angle $\theta$ using the effective moment model.

Figure 23: Dielectrophoretic force radial direction
Figure 24: Dielectrophoretic force tangential direction

Figure 25: Modulus dielectrophoretic force
For more clarification, we show the direction of the Dielectrophoretic force in different angle position.

![Diagram showing the direction of the Dielectrophoretic force in different angles.](image)

**Figure 26: Behaviour of the force in changing angle**

We can interpret the result by looking into the direction of the force vectors in figure (26), where we can see that the force is attractive in an angle of ±25° around the vertical position, whereas is repulsive for all other angles. This is consistent with the theory described in [25].
5 3D Dielectrophoretic force field

In order to understand better the behavior of the nanospheres when they are going to glide on the ground plane, we simulate on a three dimensional case an incoming particle that approaches to three fixed particle placed in triangular shape.

![Figure 27: 3D scheme](image)

5.1 Calculation in a simple case

First of all, we assume that the particle is located exactly in the vertical of the middle of the triangle. This is the simplest case talking about calculation level. Since the particle arrived from the center of the triangle, we notice that the distances between the incoming particle and the fixed particle are always the same and inversely proportional to the elevation angle.

\[ r_3 = \frac{d}{\sqrt{3} \sin \theta} \]  

(40)

In order to evaluate the total force due for each particle, we use the following formulas, obtained using the property of the tetrahedron:

\[ F_{depz} = -F_{dep} \sin \theta \cos \left( \frac{\pi}{6} \right) + F_{dep} \sin \theta \cos \left( \frac{\pi}{6} \right) \]  

(41)

\[ F_{depy} = -F_{dep} \sin \theta \sin \left( \frac{\pi}{6} \right) + F_{dep} \sin \theta \sin \left( \frac{\pi}{6} \right) + F_{dep} \sin \theta \]  

(42)

\[ F_{depz} = F_{dep} \cos \theta + F_{dep} \cos \theta + F_{dep} \cos \theta \]  

(43)
The component in the x-axis and y-axis are negligible due to the symmetry considered and the component in the direction of the z-axis as a transition from positive to negative at a given distance between the incoming particle and the three particles on the bottom substrate.

### 5.2 Obtain the others positions by Euler’s angle

Once we have calculated the force in the simplified geometry, any other direction can be calculated using the Euler’s angle rotation: yaw($\psi$), pitch($\theta$) and roll($\phi$), used also in aeronautic [26] [27].

\[
\begin{bmatrix}
F_{depx}^x \\ F_{depy}^x \\ F_{depz}^x
\end{bmatrix} =
\begin{bmatrix}
\cos \psi \cos \theta \cos \phi - \sin \psi \sin \phi \\ - \sin \psi \cos \theta \cos \phi - \cos \psi \sin \phi \\ \sin \theta \cos \phi
\end{bmatrix}
\begin{bmatrix}
\cos \psi \cos \theta \cos \phi - \sin \psi \sin \phi \\ - \sin \psi \cos \theta \cos \phi - \cos \psi \sin \phi \\ \sin \theta \cos \phi
\end{bmatrix}
\begin{bmatrix}
F_{depx} \\ F_{depy} \\ F_{depz}
\end{bmatrix}
\]

The equation above extrapolate three new cartesian coordinates relative to the rotation of the three angles. In the figures (29) and (30) show the forces in each position of the moving particle in the case that we have a distance relatively small.
We can notice that we have a change of direction of the forces when the distance between the particles become larger than $5.56 \times 10^{-7} m$, so greater than 3 times the radius.

Figure 29: 3D attractive forces

Figure 30: 3D repulsive forces
In order to calculate the influence of the Dielectrophoretic force in our system, let calculate the Weight force, using the formula (44),

\[
V_{\text{sphere}} = \frac{4}{3} \pi r_{\text{cm}}^3
\]

\[
M_{\text{ns}} = \frac{V_{\text{sphere}} \rho}{1000}
\]

\[
F_{\text{weight}} = M_{\text{ns}} g
\]  

where \( V_{\text{sphere}} \) is the volume of the nanosphere, \( r_{\text{cm}} \) is the radius of the nanosphere in cm, \( M_{\text{ns}} \) is the mass of the nanosphere in Kg, \( \rho \) is the density of the polystyrene \( (\rho = 1.05 \frac{\text{g}}{\text{cm}^3}) \), \( F_{\text{weight}} \) is the Weight force in N and \( g \) is the gravity acceleration, equal to \( 9.81 \frac{\text{m}}{\text{s}^2} \). With those formulas we obtain a Weight force equal to \( 2.5 \times 10^{-16} \) N. Comparing it to the Dielectrophoretic force, that it is of the order of \( 10^{-23} \), how we can see in the figure (28), we notice that the weight force is higher then the Dielectrophoretic force and hence a combination of these forces : weight in the downwards direction and the DEP force of varying direction are partly responsible for the experimental evidence. In this work we have concentrated on the DEP force only.
6 Conclusions

How we had saw in the pasts chapters, there are three main forces working in our system: the Coulomb force, the Weight force and the Dielectrophoretic force. With the data that we have extrapolated, we can derived those hypotesis:

1. At the beginning, when the droplets get outside the conejet, the nanospheres are wet, so the main force is the Coulomb one, toward the substrate (figures (14) (16));

2. When the particle are dried, the Coulomb force is zero, so the main force that acts in this conditions is the weight force;

3. When the particle land to the substrate, the Coulomb force still zero and the Dielectrophoretic force, with the combination of other forces like gravitational and hidrodynamic forces, explain the self-assembly saw in the empirical experiments [24].
A MATLAB CODE with explanation

%****************************
% schwartz−christofell model
%****************************
% Made by Davide Padoan− Universitat Politgecnica de Catalunya/ Politecnico
% di Torino
% calculate the field distribution in a configuration electrode
% short−plane following the equations explicated in Appl. Phys Letts ,
% 92, 173902(2008) by T.SUn, N.G. Green H.Morgan de la Universidad de
% Southampton

%DATOS
clear all;
h=10e−2;%it's the double of the distance needle−plane
h1=8e−2;
h2=12e−2;
w1=0.1e−3;
d11=4.995e−2;
d21=4.995e−2;
w2=0.5e−3;
d12=4.975e−2;
d22=4.975e−2;
w=0.3e−3;%width of the needle(diameter)
d1=4.985e−2;%half distance end to end edge of flat plate collector to ground
d2=4.985e−2;%the same but on the other side
V=10000;%potential applied at the needle, the plane is the ground
D=360e−9;%diameter of the particle
R=D/2;%radius of the particle
epsilon_vacuum=8.854187817e−12; %vacuum permittivity
epsilon_polystyrene=2.65*epsilon_vacuum;%polystirene permittivity
epsilon_air=1.00058986*epsilon_vacuum;%air permittivity
dist_max=20*R;%distance between particles
dist_10=10*R;%distance between particles

%complex plane T, every values are in the real axis
TA=0;
TB=1;
TC=1.0009;
eq1=h/(2*(d1+w+d2));

%Hilberg's approximation
if eq1>1
M= (0.25*exp(h*pi/(2*(d1+d2+w))));
k1= (M−1)/(M+1);
else
M= 0.25*exp(2*pi*(d1+d2+w)/h);
end
```matlab
kl = sqrt(1 - ((M-1)/(M+1))^2)
end
m=k1^2;
TF = (TB*(TC-TA)+k1^2-TA*(TC-TB))/((TC-TA)*k1^2-(TC-TB));
Kk = ellipke(m); %complete elliptical integral K(k1)

C3 = h/(2*Kk);
a = 0+1i*d2/C3;
[Sni,Cni,Dni] = ellipji(a,m,0.01); %call the ellipji.m file that give the
%three elliptical functions, we needs only
%sn and cn

b = 0+1i*(w+d2)/C3;
[Snibis ,Cnibis,Dnibis] = ellipji(b,m,0.01);

TE = TF*TC*Cni^2/(TC-TF*Sni^2);
TD = TF*TC*Cnibis^2/(TC-TF*Snibis^2);

k2 = sqrt((TE-TD)*(TF-TC)/((TF-TD)*(TE-TC)));
k2prima = sqrt(1-k2^2);
m2 = k2prima^2;
Kk2prima = ellipke(m2);
field = 2*V/h;

Zx = linspace(0,5e-2,100);
Zy = linspace(0,(d1+d2+w),100);

z = 1;
while (z <= 100)
    c = 1;
    while (c <= 100)
        Z = Zx(c) + 1i*Zy(z);
        [SnT(c,z),CnT(c,z),DnT(c,z)] = ellipji(Z/C3,m,0.00000000001);
        T(c,z) = (TF*TC*(CnT(c,z))^2)/(TC-TF*(SnT(c,z))^2);
        E_0(c,z) = (conj(1i*(2*V/h)*(Kk/Kk2prima)*)((T(c,z)-TB)^(0.5)*
            (TE-TC)^(0.5)/((TF-TD)^(0.5)*
            (TE-TC)^(0.5)/((TF-TB)^(0.5)*(TC-TA)^(0.5)))*
            ((T(c,z)-TE)^(0.5)*(T(c,z)-TD)^(0.5))*((T(c,z)-TA)^(0.5)/
            ((T(c,z)-TD)^(0.5)*(T(c,z)-TE)^(0.5)))));
        c = c + 1;
    end
    z = z + 1;
end

eqh1 = h1/(2*(d1+w+d2));

%Hilberg's approximation
if eqh1 >= 1
```

\[ M = \frac{0.25 \cdot \exp(h_1 \pi / (2 \cdot (d_1 + d_2 + w)))}{(M-1)/(M+1)}; \]

\[ k_1 = \frac{M - 1}{M + 1}; \]

\[ \text{else} \]

\[ M = \frac{0.25 \cdot \exp(2 \cdot \pi \cdot (d_1 + d_2 + w) / h_1)}{h_1}; \]

\[ k_1 = \sqrt{1 - \left(\frac{M - 1}{M + 1}\right)^2}; \]

\[ \text{end} \]

\[ m = k_1^2; \]

\[ TF = \frac{(T_B \cdot (T_C - T_A) \cdot k_1^2 - T_A \cdot (T_C - T_B))}{(T_C - T_A) \cdot k_1^2 - (T_C - T_B)}; \]

\[ K_k = \text{ellipke}(m); \] % complete elliptical integral \( K(k) \)

\[ C_3 = \frac{h_1}{2 \cdot K_k}; \]

\[ a = 0 + \text{1i} \cdot \frac{d_2}{C_3}; \]

\[ [Sni, Cni, Dni] = \text{ellipji}(a, m, 0.01); \] % call the ellipji.m file that give the \% three elliptical functions, we needs only \% sn and cn

\[ b = 0 + \text{1i} \cdot \frac{(w + d_2)}{C_3}; \]

\[ [Snibis, Cnibis, Dnibis] = \text{ellipji}(b, m, 0.01); \]

\[ TE = \frac{TF \cdot T_C \cdot Cni^2}{(T_C - TF \cdot Sni^2)}; \]

\[ TD = \frac{TF \cdot T_C \cdot Cnibis^2}{(T_C - TF \cdot Snibis^2)}; \]

\[ k_2 = \sqrt{(TE - TD) \cdot (TF - TC) / ((TF - TD) \cdot (TE - TC))}; \]

\[ k_2prima = \sqrt{1 - k_2^2}; \]

\[ m_2 = k_2prima^2; \]

\[ K_k2prima = \text{ellipke}(m_2); \]

\[ field = 2 \cdot V/h_1; \]

\[ Zxh1 = \text{linspace}(0, 4 \cdot 10^{-2}, 100); \]

\[ z = 1; \]

\[ \text{while (z < 100)} \]

\[ c = 1; \]

\[ \text{while (c < 100)} \]

\[ Z = Zxh1(c) + \text{1i} \cdot Z_{y}(z); \]

\[ [SnT(c, z), CnT(c, z), DnT(c, z)] = \text{ellipji}(Z / C_3, m, 0.000000000001); \]

\[ T(c, z) = \frac{(TF \cdot TC \cdot (T_{C} (c, z))^2)}{(TC - TF \cdot (SnT(c, z)) \cdot 2)}; \]

\[ E_{Oh1}(c, z) = \text{conj} \left( \text{i} \cdot (2 \cdot V/h_1) \cdot (K_k / K_k2prima) \cdot ((TF - TD)^0.5) \cdot \text{TE} - TC) \cdot (0.5) / ((TF - TB)^0.5) \cdot (TC - TA)^0.5 \right) \cdot ((T(c, z) - TB)^0.5) \cdot (T(c, z) - TE)^0.5; \]

\[ c = c + 1; \]

\[ end \]

\[ z = z + 1; \]

\[ end \]

\[ eqh21 = \frac{h_2}{(2 \cdot (d_1 + w + d_2))}; \]
if eqh21 = 1
    M = (0.25 * exp(h2 * pi / (2 * (d1 + d2 + w))));
    k1 = (M - 1) / (M + 1);
else
    M = 0.25 * exp(2 * pi * (d1 + d2 + w) / h2);
    k1 = sqrt(1 - ((M - 1) / (M + 1)) ^ 2);
end
m = k1 ^ 2;
TF = (TB * (TC - TA) * k1 ^ 2 - TA) / ((TC - TA) * k1 ^ 2 - (TC - TB));
Kk = ellipke(m); % complete elliptical integral K(k1)

C3 = h2 / (2 * Kk);
a = 0 + 1i * d2 / C3;
[Sni, Cni, Dni] = ellipji(a, m, 0.01); % call the ellipji.m file that give the
% three elliptical functions, we needs only
% sn and cn

b = 0 + 1i * (w + d2) / C3;
[Snibis, Cnibis, Dnibis] = ellipji(b, m, 0.01);

TE = TF * TC * Cni ^ 2 / (TC - TF * Snibis ^ 2);
TD = TF * TC * Cnibis ^ 2 / (TC - TF * Snibis ^ 2);
k2 = sqrt((TE - TD) * (TF - TC) / ((TF - TD) * (TE - TC)));
k2prima = sqrt(1 - k2 ^ 2);
m2 = k2prima ^ 2;
Kk2prima = ellipke(m2);
field = 2 * V / h2;
Zxh2 = linspace(0, 6e-2, 100);

z = 1;
while (z < 100)
    c = 1;
    while (c <= 100)
        Z = Zxh2(c) + 1i * Zy(z);
        [SnT(c, z), CnT(c, z), DnT(c, z)] = ellipji(Z / C3, m, 0.000000000001);
        T(c, z) = (TF * TC * (CnT(c, z)) ^ 2) / (TC - TF * (SnT(c, z)) ^ 2);
        E0h2(c, z) = conj(1i * (2 * V / h2) * (Kk / Kk2prima) * (TF - TD) ^ (0.5) * ...
                        (TE - TC) ^ (0.5) / ((TF - TB) ^ (0.5) * (TC - TA) ^ (0.5)) * ...
                        (T(c, z) - TA) ^ (0.5) / ((T(c, z) - TD) ^ (0.5) * (T(c, z) - TE) ^ (0.5)))
                        )
        c = c + 1;
    end
    z = z + 1;
end
\[\text{eqw11} = \frac{h}{2 \cdot (d11 + w1 + d21)};\]

**Hilberg's approximation**

\[\text{if } \text{eqw11} > 1\]

\[\begin{align*}
M &= \frac{0.25 \cdot \exp \left( \frac{h \cdot \pi}{2 \cdot (d11 + d21 + w1)} \right)}{M-1}\left(M+1\right); \\
k1 &= \sqrt{1 - \left(\frac{M-1}{M+1}\right)^2};
\end{align*}\]

\[\text{else}\]

\[\begin{align*}
M &= \frac{0.25 \cdot \exp \left( 2 \cdot \pi \cdot (d11 + d21 + w1) / h \right)}{M-1}\left(M+1\right); \\
k1 &= \sqrt{1 - \left(\frac{M-1}{M+1}\right)^2};
\end{align*}\]

\[\text{end}\]

\[m = k1^2;\]

\[\text{TF} = \frac{(TB \cdot (TC - TA) \cdot k1^2 - TA \cdot (TC - TB))}{(TC - TA \cdot k1^2 - (TC - TB));}\]

\[Kk = \text{ellipke}(m); \quad \text{%complete elliptical integral } K(k1)\]

\[C3 = \frac{h}{2 \cdot Kk};\]

\[a = 0 + \frac{1i \cdot d21}{C3};\]

\[[Sni, Cni, Dni] = \text{ellipji}(a, m, 0.01); \quad \text{%call the ellipji.m file that give the}\]

\[\text{three elliptical functions, we needs only } \text{sn and cn}\]

\[b = 0 + \frac{1i \cdot (w1 + d21)}{C3};\]

\[[Snibis, Cnibis, Dnibis] = \text{ellipji}(b, m, 0.01);\]

\[\text{TE} = \frac{TF \cdot TC \cdot Cni^2}{(TC - TF \cdot Sni^2)};\]

\[\text{TD} = \frac{TF \cdot TC \cdot Cnibis^2}{(TC - TF \cdot Snibis^2)};\]

\[k2 = \sqrt{\frac{(TE - TD) \cdot (TF - TC)}{(TF - TD) \cdot (TE - TC)}};\]

\[k2prima = \sqrt{1 - k2^2};\]

\[m2 = k2prima^2;\]

\[Kk2prima = \text{ellipke}(m2);\]

\[\text{field} = 2 \cdot V / h;\]

\[\text{Zx} = \text{linspace}(0, 5e-2, 100);\]

\[\text{Zy1} = \text{linspace}(0, (d11 + d21 + w1), 100);\]

\[z = 1;\]

\[\text{while } (z <= 100)\]

\[c = 1;\]

\[\text{while } (c <= 100)\]

\[Z = \text{Zx}(c) + 1i \cdot \text{Zy}(z);\]

\[\begin{align*}
[SniT(c, z), CnT(c, z), DnT(c, z)] &= \text{ellipji}(Z/C3, m, 0.000000000001); \\
T(c, z) &= \frac{(TF \cdot TC \cdot (CnT(c, z))^2)}{(TC - TF \cdot (SnT(c, z))^2)}; \\
E_{01w1}(c, z) &= \text{conj}(1i \cdot (2 \cdot V / h) \cdot (Kk / Kk2prima) \cdot (\text{TF} - \text{TD}) \cdot (0.5) \cdot (\text{TE} - \text{TC}) \cdot (0.5) / ((\text{TF} - \text{TB}) \cdot (0.5) \cdot (\text{TC} - \text{TA}) \cdot (0.5)) \cdot ((T(c, z) - \text{TB}) \cdot (0.5) \cdot (\text{TE} - \text{TC}) \cdot (0.5)) \cdot ((T(c, z) - \text{TA}) \cdot (0.5)) \cdot ((\text{TF} - \text{TD}) \cdot (0.5) \cdot (\text{TE} - \text{TC}) \cdot (0.5)) \cdot ((\text{TF} - \text{TB}) \cdot (0.5) \cdot (\text{TC} - \text{TA}) \cdot (0.5)) \cdot ((T(c, z) - \text{TB}) \cdot (0.5));
\end{align*}\]
\[
(T(c,z)-TA)^{(0.5)/((T(c,z)-TD)^{(0.5)}*(T(c,z)-TE)^{(0.5)})})
\]

c=c+1;
end

z=z+1;
end

eqw21=h/(2*(d12+w2+d22));

\text{%Hilberg's approximation}

\text{if } eqw21 > 1
\text{M} = (0.25*exp(h*pi/(2*(d12+d22+w2))));
\text{k1} = (M-1)/(M+1);
\text{else}
\text{M} = 0.25*exp(2*pi*(d12+d22+w2)/h);
\text{k1} = sqrt(1-(M-1)/(M+1))^2);
\text{end}

\text{m=k1^2;}
\text{TF} = (TB*(TC-TE)*k1^2-TE*(TB-TC))/((TC-TE)*k1^2-(TC-TB));
\text{Kk=ellipke(m); %complete elliptical integral K(k1)}

C3=h/(2*Kk);

\text{a=0+1i*d22/C3;}

[Snii,Cnii,Dnii]=ellipji(a,m,0.01); %call the ellipji.m file that give the
two elliptical functions, we needs only
\text{sn and cn}

b=0+1i*(w2+d22)/C3;

[Snibis,Cnibis,Dnibis]=ellipji(b,m,0.01);

TE= TF*TC*Cnii^2/(TC-TF*Snii^2);
TD=TF*TC*Cnibis^2/(TC-TF*Snibis^2);

k2=sqrt(((TE-TD) *(TF-TC))/((TF-TD) *(TE-TC)));

k2prima=sqrt(1-k2^2);

m2=k2prima^2;

Kk2prima=ellipke(m2);

field=2*V/h;

Zx=linspace(0,5e-2,100);
Zy2=linspace(0,(d12+d22+w2),100);

z=1;
\text{while (z<100)
\text{c}=1;
\text{while (c<100)
\[ \begin{align*}
Z &= Zx(c) + 1i*Zy(z); \\
|S_{nT}(c,z), C_{nT}(c,z), D_{nT}(c,z)| &= \text{ellipji}(Z/C3, m, 0.00000000001); \\
T(c,z) &= \frac{(TF*TC*(C_{nT}(c,z))^2)}{(TC-TF*(S_{nT}(c,z))^2)}; \\
E_{0w2}(c,z) &= \text{conj}(1i*(2*V/h)*(Kk/Kk^2prima)*((TF-TD)^0.5)*... \\
&\quad ((TE-TC)^0.5)/((TF-TB)^0.5)*((TC-TA)^0.5))*((T(c,z)-TB)^0.5)*... \\
&\quad ((T(c,z)-TA)^0.5)/((T(c,z)-TD)^0.5)*((T(c,z)-TE)^0.5))); \\
c &= c+1; \\
\end{align*} \]

end
z=z+1;
end

figure(20)
plot(Zy, abs(E_{0h1}(62,:)), 'b', Zy, abs(E_{0}(50,:)), 'r', Zy, abs(E_{0h2}(42,:)), 'g');
legend('h=8cm', 'h=10cm', 'h=12cm')
title('Behaviour Electric Field with h variation (measured in 2.5 cm)');
xlabel('Distance(m)');
ylabel('Absolute Electric Field(V/m)');

figure(21)
plot(Zy, abs(E_{0w1}(50,:)), 'b', Zy, abs(E_{0}(50,:)), 'r', Zy, abs(E_{0w2}(50,:)), 'g');
legend('w=0.1mm', 'w=0.3mm', 'w=0.5mm')
title('Behaviour Electric Field with w variation (measured in 2.5 cm)');
xlabel('Distance(m)');
ylabel('Absolute Electric Field(V/m)');

EA = abs(E_{0});
figure(1)
plot(Zy, EA(20,:), 'b', Zy, EA(30,:), 'g', Zy, EA(40,:), 'r', Zy, EA(50,:), 'm', ...
Zy, EA(60,:), 'c', Zy, EA(70,:), 'y', Zy, EA(80,:), 'k');
legend('1 cm', '1.5 cm', '2 cm', '2.5 cm', '3 cm', '3.5 cm', '4 cm')
title('Absolute Electric Field of the system')
xlabel('Distance(m)');
ylabel('Absolute Electric Field(V/m)');

figure(17)
plot(Zx, EA(:,50), 'b');
legend('On the needle');
title('Absolute Electric Field of the system')
xlabel('Distance h(m)');
ylabel('Absolute Electric Field(V/m)');

figure(19)
plot(Zy, EA(1,:), 'b');
legend('0.05 cm');
title('Absolute Electric Field near the needle')
xlabel('Distance(m)');
ylabel('Absolute Electric Field(V/m)');

E_{cone} = EA(100,50); % electric field at 500um
[gradEx1, gradEy1] = gradient(EA);
\[ (\text{gradEx}, \text{gradEy}) = \text{gradient}(E A^2); \]

% we change the sign of the equations because the Matlab's gradient no take
% care of that

c = 1;

while \( c \leq 50 \)
    \( \text{gradEx1}(:,c) = -\text{gradEx1}(:,c); \)
    \( \text{gradEy1}(:,c) = -\text{gradEy1}(:,c); \)
    \( \text{gradEx}(:,c) = -\text{gradEx}(:,c); \)
    \( \text{gradEy}(:,c) = -\text{gradEy}(:,c); \)
    \( c = c + 1; \)
end;

figure(18)
plot(Zx, gradEx1(:,50), '−b');
legend('On the needle');
title('Electric Field gradient on the needle')
xlabel('Distance h(m)')
ylabel('Electric Field gradient(V/m)')

\[
F_{\text{depx}} = 2 \pi \epsilon_{\text{air}} R^3 \left( \frac{(\epsilon_{\text{polystyrene}} - \epsilon_{\text{air}})}{\epsilon_{\text{polystyrene}} + 2 \epsilon_{\text{air}}} \right) \text{gradEx};
\]

\[
F_{\text{depy}} = 2 \pi \epsilon_{\text{air}} R^3 \left( \frac{(\epsilon_{\text{polystyrene}} - \epsilon_{\text{air}})}{\epsilon_{\text{polystyrene}} + 2 \epsilon_{\text{air}}} \right) \text{gradEy};
\]

% taylor's cone and droplet charge

\( \rho_{\text{o}} = 1000; \ \text{Kg/m}^3 \)

\( \text{Vagua} = 73e^{-3}; \)

\( \text{theta} = 43.5; \)

\( \text{Ut} = 0.68 \text{sqrt} \left( \text{Vagua} h / \epsilon_{\text{vacuum}} \right); \)

\( \text{Ut} = 0.6791 \text{sqrt} \left( 0.02275 h / \epsilon_{\text{vacuum}} \right); \)

\( \text{flow rate} = 6.1e-10; \ \text{m}^3/s \)

\( \text{rdrop} = (\text{ro} / (4 \pi^2 \text{Vagua} \tan(\pi/2-theta) * ((V/Ut)^2-1))^{1/3} * \text{flow rate}^{2/3}; \)

\( Q = 8 \pi \text{sqrt} (\epsilon_{\text{air}} \text{V} \times \text{rdrop}^3); \)

\( FA = Q \times EA; \)

\( Fx = Q \times \text{real}(E_0); \)

\( Fy = Q \times \text{imag}(E_0); \)

\( \text{Fdep} = \text{abs}(F\text{depx} + 1i \times F\text{depy}); \)

figure(2)
plot(Zy, FA(50,:), '−b', Zy, FA(60,:), '−g', Zy, FA(70,:), '−r', ...
    Zy, FA(80,:), '−m', Zy, FA(90,:), '−c', Zy, FA(100,:), '−k')

title('Absolute Coulomb Force for a single particle')
legend('2.5 cm', '3 cm', '3.5 cm', '4 cm', '4.5 cm', '5 cm')
xlabel('Distance(m)')
ylabel('Absolute Coulomb Force(N)')

figure(3)
plot(Zy, Fdep(70,:), '−b', Zy, Fdep(80,:), '−g', Zy, Fdep(90,:), '−r', ...
    Zy, Fdep(100,:), '−k')
% calculation of force between two particles
rd=linspace(0,dist,10,26); %distance between two particles
t=1:4
r=linspace(0,dist,10,25)
alphad=linspace(0,pi/2,26); %angle between two particles
alpha=linspace(0,pi/2,25);
k=(epsilon-polystyrene-epsilon-air)/(epsilon-polystyrene+2*epsilon-air);

z=1;
while (z<25)
c=1;
while (c<26)
f=(1/D)/(sqrt(r(z)^2+(D^2)/4-r(z)*D*cos(alphad(c))));
f_d=(1/D)/(sqrt(r(z)^2+(D^2)/4+r(z)*D*cos(alphad(c))));
c=c+1;
end
z=z+1;
end
z=1;
while (z<26)
c=1;
while (c<25)
f=(1/D)/(sqrt(rd(z)^2+(D^2)/4-rd(z)*D*cos(alpha(c))));
f_d=(1/D)/(sqrt(rd(z)^2+(D^2)/4+rd(z)*D*cos(alpha(c))));
c=c+1;
end
z=z+1;
end

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c=c+1;
end
z=z+1;
end

c=1;
while (c<=26)
Pb(xhr(c,:))=4.*pi.*epsilon_vacuum.*R.*EA(100,50).*cos(alpha).*... 
(1./fxhr(:,c))' + (cos(alpha)-R.*cos(alpha).*... 
f_dr,xhr(:,c))./f,xhr(:,c)'./R.*cos(alpha).*f_dr,xhr(:,c)'-... 
(epsilon_polystyrene./epsilon_air).*f,xhr(:,c)'.*cos(alpha));
V,xhr(c,:)=((Pb,xhr(c,:)./(4.*pi.*epsilon_vacuum)).*f,xhr(:,c)';
c=c+1;
end;
c=1;
while (c<=25)
Ert(:,c)=diff(V,xr(:,c))./(dist_10/25);%we have a change of the sign
%caused by the Matlab's
%differentiation
end;
c=1;
while (c<=25)
Ert(:,c)=(EA(100,50).*cos(alpha))' + Ert(c,:)';
Pbxrxt(c,:)=4.*pi.*epsilon_vacuum.*R.*EA(100,50).*cos(alphad).*... 
(1./fxtr(:,c))' + (cos(alphad)-R.*cos(alphad).*... 
f_dr,xtr(:,c))./f,xtr(:,c)'./R.*cos(alphad).*f_dr,xtr(:,c)'-... 
(epsilon_polystyrene./epsilon_air).*f,xtr(:,c)'.*cos(alphad));
V,xtr(c,:)=((Pb_xt(c,:)./(4.*pi.*epsilon_vacuum)).*f,xtr(:,c)';
Ealpha_sinxr(c,:)=-diff(V,xr(c,:))./(pi/2/25);
Ealpha(c,:)=(EA(100,50).*sin(alpha)) + Ealpha_sinxr(c,:)/r(c);
c=c+1;
end;

Eabs=sqrt(Er.'^2+Ealpha.'^2);
[gradEr,gradEalpha]=gradient(Eabs.'^2);
Fdepr=2.*pi.*epsilon_air.*R.^3.*k.*gradEr./(dist_10/25);
Fdepalpha=2.*pi.*epsilon_air.*R.^3.*k.*gradEalpha./(pi/2/25);
c=1;
while (c<=25)
z=1;
while (z<=25)
if Fdepr(c,z)>0
phi(c,z)=atan(Fdepalpha(c,z)/Fdepr(c,z));
else
phi(c,z)=atan(Fdepalpha(c,z)/Fdepr(c,z)) + pi;
end;
end;
end;
z=z+1;
end;
c=c+1;
end;
asx=r(25).*sin(alpha);
asy=r(25).*cos(alpha);
Fx=sqrt(Fdepr(:,25)'.^2+Fdepalpha(:,25)'.^2).*cos((pi/2-alpha-phi(:,25)));
Fy=sqrt(Fdepr(:,25)'.^2+Fdepalpha(:,25)'.^2).*sin((pi/2-alpha-phi(:,25)));
title('Absolute Dielectrophoretic Force')
xlabel('theta(degrees)')
ylabel('Absolute Dielectrophoretic Force(N)')
figure(10)
angle=(alpha'+(pi/2-phi(:,25))).*180/pi;
plot(alphag,angle,'-k')
title('phi angle')
xlabel('theta(degrees)')
ylabel('phi(degrees)')

%calculation forces between 3 to 1 (3D) with particle in the middle
%distance 20*R
alpha_min=atan(sqrt(3)/30);
alpha_max=atan(sqrt(3)/3);
alpha=linspace(alpha_min,alpha_max,25); %angle between two particles
alphad=linspace(alpha_min,alpha_max,26); %angle between two particles
alphadd=linspace(alpha_min,alpha_max,27); %angle between two particles
alphag=alpha.*180/pi;
R_cm=R*10^2; %Radius in cm
Volume_sphere=4/3*pi*R_cm^3;
dens=1.05; % density polystirene in g/cm^3
weight=Volume_sphere*dens/1000; %in kg
F_weight=weight*9.81;
c=1;
while (c<=25)
    r3g(c)=D*sqrt(3)/(3*sin(alpha(c)));%distance between spheres
    c=c+1;
end;
c=1;
while (c<=26)
    r3(c)=D*sqrt(3)/(3*sin(alphad(c)));%distance between spheres
    c=c+1;
end;
c=1;
while (c<=27)
    rd3(c)=D*sqrt(3)/(3*sin(alphadd(c)));%distance between spheres
    c=c+1;
end;
z=1;
while (z<=27)
    c=1;
    while (c<=27)
        if z==28-c
            f(c)=(1/D)/(sqrt(rd3(z)^2+(D^2)/4-rd3(z)*D*cos(alphadd(c))))-
            (1/D)/(sqrt(rd3(z)^2+(D^2)/4+rd3(z)*D*cos(alphadd(c))));
            f_dr(c)=-((2*rd3(z)-D*cos(alphadd(c)))/(2*D*sqrt(rd3(z)^2+
                D^2)/4-rd3(z)*D*cos(alphadd(c))))/rd3(z)^2+(D^2)/4-
                (rd3(z)^2+(D^2)/4+rd3(z)*D*cos(alphadd(c))))/rd3(z)^2+(D^2)/4+
                rd3(c)*D*cos(alphadd(c)));
        end;
        c=c+1;
    end;
    c=c+1;
end;
end
z=z+1;
end

Pb=4.*pi.*epsilon_vacuum.*R.*EA(100,50).*cos(alphadd).*\(1/f+\)
\((cos(alphadd)−(R.*cos(alphadd).*f.dr)/f)/(R.*cos(alphadd).*f.dr−\)
\((epsilon_polsyrene./epsilon_air).*f.*cos(alphadd)))
V=(Pb./(4.*pi.*epsilon_vacuum)).*f;
E_r_t=D.*cos(alphad).*sqrt(3)./(3.*sin(alphad).^2).*diff(V)/...
\((abs(alpha(25)−alpha(1))/25)\);
E_r3=(EA(100,50).*cos(alphad)) + E_r_t;
E_alpha_sin_r=diff(V)./(abs(alpha(25)−alpha(1))/25);
E_alpha3=−(EA(100,50).*sin(alphad))+E_alpha_sin_r./r3;
E_abs3=sqrt(E_alpha3.^2+E_r3.^2);

gradEr3=D.*cos(alpha).*sqrt(3)./(3.*sin(alpha).^2).*diff(E_abs3.^2)/...
\((abs(alpha(25)−alpha(1))/25)\);
gradEalpha3=diff(E_abs3.^2)./(abs(alpha(25)−alpha(1))/25);
Fdepalpha3=2*pi*epsilon_air*R.^3*k*gradEalpha3;
Fdepr3=2*pi*epsilon_air*R.^3*k*gradEr3;
Fdepabs3=sqrt(Fdepalpha3.^2+Fdepr3.^2);
c=1;
while (c<25)
if Fdepr3(c)>0
 phi3(c)=atan(Fdepalpha3(c)/Fdepr3(c));
else
 phi3(c)=atan(Fdepalpha3(c)/Fdepr3(c))+pi;
end;
c=c+1;
end;

Fdepx=−(Fdepabs3.^cos(pi/6)+Fdepabs3.^cos(pi/2-alpha+phi3); Fdepy=−(Fdepabs3.^sin(pi/6)−Fdepabs3.^sin(pi/2-alpha+phi3);
Fdepz=(Fdepabs3.^cos(alpha)+Fdepabs3.^cos(alpha)+Fdepabs3.^cos(alpha)).*
\(\sin(pi/2−alpha+phi3)\);
Fdep_dip_xy=Fdepabs3.*cos(pi/2−alpha+phi3);
Fdep_dip_z=Fdepabs3.*sin(pi/2−alpha+phi3);
alphag=alpha.*180./pi;
figure(11)
pplot(r3g,Fdepx)
title('Absolute Dielectrophoretic Force in x')
xlabel('Distancia(m)')
ylabel('Absolute Dielectrophoretic Force in x(N)')

figure(12)
pplot(r3g,Fdepy)
title('Absolute Dielectrophoretic Force in y')
xlabel('Distancia(m)')
ylabel('Absolute Dielectrophoretic Force in y(N)')

figure(13)
plot(r3g,Fdepz)
title('Absolute Dielectrophoretic Force in z')
xlabel('Distancia (m)')
ylabel('Absolute Dielectrophoretic Force in z (N)')

% threshold electric field
k_b = 1.3806488*10^(-23); % Boltzmann's constant
T = 300; % Room temperature in Kelvin
Eth = 1.7*R^(-3/2)*sqrt(k_b*T/epsilon_air)/k;

% 1 to 3 with moving particle using Euler's angles
asse_x = 1;
asse_y = 2;
asse_z = 3;
Yaw = linspace(-pi/4, pi/4, 12); % (psi)
Pitch = linspace(-pi/4, pi/4, 12); % (theta)
Roll = linspace(-pi, pi, 12); % (phi)
angolo = 17; % 5

[Y, RO] = meshgrid(yaw, roll);
Fdep1 = [-Fdep_dip_xy(angolo).*sin(alpha(angolo)).*cos(pi/6+pi/3);...
        -Fdep_dip_xy(angolo).*sin(alpha(angolo)).*sin(pi/6+pi/3);...
        Fdep_dip_z(angolo).*cos(alpha(angolo))];
Fdep2 = [-Fdep_dip_xy(angolo).*sin(alpha(angolo)).*cos(pi/3);...
        Fdep_dip_xy(angolo).*sin(alpha(angolo)).*cos(pi/3);...
        Fdep_dip_z(angolo).*cos(alpha(angolo))];
Fdep3 = [Fdep_dip_xy(angolo).*sin(alpha(angolo)).*cos(pi/3);...
        -Fdep_dip_dip_xy(angolo).*sin(alpha(angolo)).*sin(pi/3);...
        Fdep_dip_z(angolo).*cos(alpha(angolo))];

Fx1 = Fdep1(asse_x);
Fy1 = Fdep1(asse_y);
Fz1 = Fdep1(asse_z);
Fx2 = Fdep2(asse_x);
Fy2 = Fdep2(asse_y);
Fz2 = Fdep2(asse_z);
Fx3 = Fdep3(asse_x);
Fy3 = Fdep3(asse_y);
Fz3 = Fdep3(asse_z);

[P, RO] = meshgrid(pitch, roll);
%cambio coordinate
k = 1;
while k <= 12
    l = 1;
    while l <= 12
        g = 1;
        ...
while g<=12
    Fdep1Ex(g,l,k)=((cos(yaw(g)).*cos(pitch(l))).*cos(roll(k))−...
        sin(yaw(g)).*sin(roll(k))) +...
        sin(yaw(g)).*cos(pitch(l)).*cos(roll(k)) +...
        cos(yaw(g)).*sin(roll(k)) −...
        sin(pitch(l)).*cos(roll(k))).*F1x;
    Fdep1Ey(g,l,k)=((-cos(yaw(g)).*cos(pitch(l))).*sin(roll(k))−...
        sin(yaw(g)).*sin(roll(k)))−...
        sin(yaw(g)).*cos(pitch(l)).*sin(roll(k)) +...
        cos(yaw(g)).*cos(roll(k)) +...
        sin(pitch(l)).*sin(roll(k))).*F1y;
    Fdep1Ez(g,l,k)=(cos(yaw(g)).*sin(pitch(l)) +...
        sin(yaw(g)).*sin(pitch(l)) + cos(pitch(l))).*F1z;
    g=g+1;
end;
l=l+1;
end;
k=k+1;
end;

k=1;
while k<=12
    l=1;
    while l<=12
        g=1;
        while g<=12
            X=([cos(yaw(g)).*cos(pitch(l))].*cos(roll(k))−...
                sin(yaw(g)).*sin(roll(k)));
        g=g+1;
    l=l+1;
end;
k=k+1;
end;
\[
\sin(yaw(g)) \cdot \cos(pitch(l)) \cdot \cos(roll(k)) + \cdots \\
\cos(yaw(g)) \cdot \sin(roll(k)) - \sin(pitch(l)) \cdot \cos(roll(k)) - \cdots \\
(-\cos(yaw(g)) \cdot \cos(pitch(l)) \cdot \sin(roll(k)) - \cdots \\
\sin(yaw(g)) \cdot \cos(roll(k))) - \cdots \\
-\sin(yaw(g)) \cdot \sin(pitch(l)) \cdot \cos(roll(k)) + \cdots \\
\cos(yaw(g)) \cdot \sin(roll(k)) + \sin(pitch(l)) \cdot \sin(roll(k)) \\
\cos(yaw(g)) \cdot \sin(pitch(l)), + \sin(yaw(g)) \cdot \sin(pitch(l)) + \cdots \\
+ \cos(pitch(l))) \cdot 10 \cdot R;
\]

\[F_{depetotEx}(g,l,k) = F_{dep1Ex}(g,l,k) + F_{dep2Ex}(g,l,k) + F_{dep3Ex}(g,l,k) ;
\]

\[F_{depetotEy}(g,l,k) = F_{dep1Ey}(g,l,k) + F_{dep2Ey}(g,l,k) + F_{dep3Ey}(g,l,k) ;
\]

\[F_{depetotEz}(g,l,k) = F_{dep1Ez}(g,l,k) + F_{dep2Ez}(g,l,k) + F_{dep3Ez}(g,l,k) ;
\]

\[ejex(g,l,k) = X(1,1) + X(2,1) + X(3,1);
\]

\[ejey(g,l,k) = X(1,2) + X(2,2) + X(3,2);
\]

\[ejez(g,l,k) = X(1,3) + X(2,3) + X(3,3);
\]

\[g = g + 1;
\]

\[l = l + 1;
\]

\[k = k + 1;
\]

\[end;
\]

\[\text{figure}(47)\]
\[\text{quiver3}(ejex,ejy,ejej,F_{depetotEx},F_{depetotEy},F_{depetotEz});\]

\[\text{title}('Direction Dielectrophoretics Forces');\]

\[\text{xlabel}('eje x(m)');\]
\[\text{ylabel}('eje y(m)');\]
\[\text{zlabel}('eje z(m)');\]
References

[1] R. Daz, S. Payen, *Biological cell separation using dielectrophoresis in a microfluidic device*, University of California, Berkeley, Bio and Thermal Engineering Laboratory EECS 245


[7] Product Info Sheet - Schoeller Textiles AG


