Modelling of a Liquid Desiccant Electrospray in an Evaporative Cooler Dehumidifier for Tertiary Hospitals Using Computational Fluid Dynamics

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Abstract

The climate in a hospital's operating theatre in terms of temperature, air flow and humidity affects medical personnel's working conditions and the healing process for patients. Evaporative cooling technology is a sustainable option whose latent load can be handled desiccant dehumidification. The combination of a liquid desiccant and electro-hydrodynamic techniques to produce small droplets with increased surface contact for humidity reduction is commendable. Accordingly, this study is centered on developing Computational Fluid Dynamics simulations in ANSYS FLUENT for electrospray modelling. A numerical code is developed to simultaneously solve the coupled electrohydrodynamic and electrostatic equations and determine the shape of cone jet as an effect of the applied electric field for a glycerol electrospray in an air dehumidification system. The Volume of Fluid model of CFD FLUENT and Melcher-Taylor leaky dielectric model was established. The CFD model developed does not include a droplet break-up and the dynamics of droplet evaporation.

Keywords
Hospital Operating Theatre, Evaporative Cooling, Electrospray, CFD model, cone jet.

1. Introduction

The microclimate in hospitals disturbs working conditions of the medical personnel and healing process for patients under treatment. To ensure a conducive healing climate, Zimbabwe's tertiary hospitals employ vapour compression based systems, (VCS), to condition air as per tradition (Ascione et al., 2013) but these have been condemned of their considerable dependency on electricity (Tao, et al 2019). This is so because the sensible and latent heat load are handled by cooling air below due point which at times may require reheating to achieve required temperature. The use of ozone layer depleting and global warming chlorofluorocarbons (CFCs) and hydrofluorocarbons (HFCs) based refrigerants in VCS is disturbing. The unsustainability of these systems has pushed for the development of sustainable green air conditioning system technologies in which sensible and latent heat loads can be handled separately (Tao, et al, 2019).

Evaporative cooling technology is non-polluting and energy efficient (Oliveira et al., 2000; Buker and Riffat, 2016; Rafique et al., 2015; Peng et al., 2015; Teke and Timur, 2014). The sensible load is removed by evaporating the water on a pad using the air's sensible heat as it passes through a wetted pad using a quarter of VCS's energy (Rafique et al., 2015; Khoukhi, 2013; Luo et al., 2016; Rong et al., 2017) and water (R718) as refrigerant which is non-polluting (Maurya, et al, 2014).

The latent load in form of extra water in processed air is a challenge in humid and tropical climates like Zimbabwe's, (Guan, et al, 2015). This latent load after evaporative cooling can be handled by electrochemical and desiccant dehumidification (Jain, et al, 1994; Fakhrabadi and Kowsary, 2016). Solid desiccant technology have proved to be inefficient and consume high energy (Fakhrabadi and Kowsary, 2016; O'Connor, et al 2016) thus research is looking at developing efficient liquid desiccant systems, (Figure 1); (Salazar et al., 2018; Jain, et al, 1994) due to their precise humidity regulation capacity and great energy savings (Tao, et al, 2019).

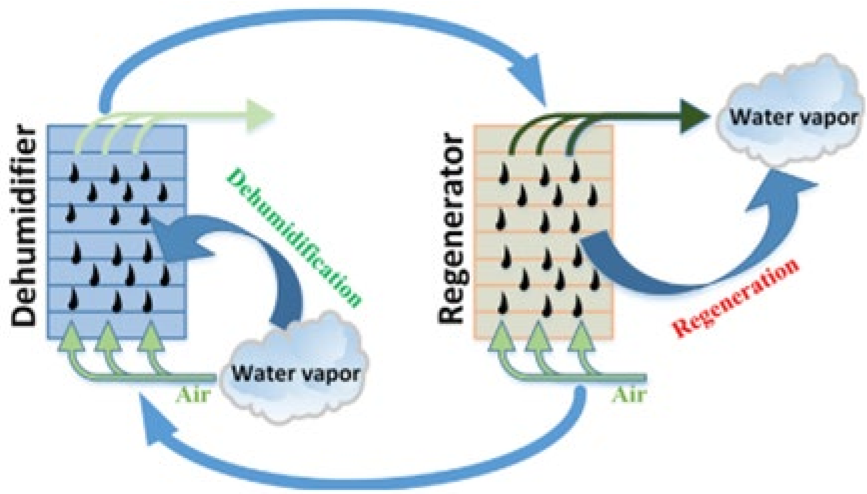

Figure 1: Liquid desiccant dehumidification schematic diagram ((Tao, et al, 2019)

Liquid desiccant system performance is based on water mass transfer from the air to the desiccant material. Several technologies including falling film towers have been developed to enhance system's performance, (O'Connor, et al, 2016; Kinsara, Elsayedt and Arabia, 1996; Dai *et al.*, 2001) but poor contact surface was realised. When desiccant droplet diameter is decreased, contact surface area is increased (Salazar *et al.*, 2018). Electrospraying is such a technique which generates uniform nano-droplets (Eslamian and Shekarriz, 2009) yielding moisture over an air stream (López-Herrera *et al.*, 2004) and the concept is as presented in Figure 2. As defined by Jaworek *et al.*, (2009) electrospraying is a low-energy process in which a nozzle is brought about after stress has been exerted by electric field on the surface of a liquid flowing resulting in the jets becoming fine droplets due to the repulsive Coulomb forces. Needles are used for the production of micrometre and submicrometre dimension of particles and the liquid should have very low flow rates and high electrical conductivity hence a single emitter is inadequate, (Parhizkar *et al.*, 2017). Multiplexed electrospray setups solve the problem and these have been primarily investigated by several researchers including by Bocanegra *et al.*, (2005) and Parhizkar *et al.*, (2017) who integrated multi-injectors. Salazar *et al.*, (2018), evaluated the use of the technique for application in hospital theatre rooms.

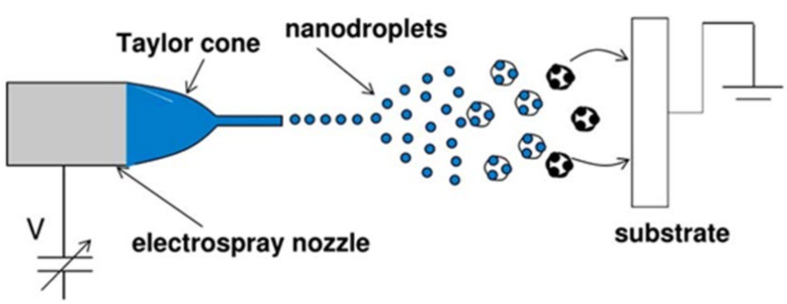

Figure 2: Electrospray technique in spray pyrolysis/drying, (Eslamian and Shekarriz, 2009)

Several work has been done to investigate the electrospray process and Zeng, et al, (no date) modelled electrospray with Melcher and Taylor's leaky-dielectric liquid theory using VOF of FLOW 3D to design a µfluidic device. Lastow and Balachandran [30] simulated electrospray using VOF of CFX 4.4. Wu, et al (2012) used FLOW 3D of CFD to simulate emitter designs with a maximum of three emitters. Gałeka and Strzelczyk, (2019), investigated experimentally and numerically the velocity profiles of an electrohydrodynamic flow generator adopting Multiphysics Object-Oriented Simulation Environment (MOOSE) framework for simulations. Parhizkar *et al.*, (2017) investigated the performance of a multi-jet electrospray system for large scale throughput in production of polymeric micro/nanoparticles through experiments and found that throughput can be increased.

Salazar *et al.*, (2018) did a technical feasibility study of the electrospray technique in the production of small droplets of desiccant liquids for humidity control. They assessed suitability of liquid desiccant material for air conditioning, and concluded that ionic liquids, with $EMIBF_4$ included doesn't perform well like alcohols such as glycerol in dehumidification, (Salazar *et al.*, 2018). Glycerol, is a non-toxic, non-irritant, biodegradable, recyclable alcohol which has very high boiling point, low vapor pressure and is stable under normal conditions which have been shown experimentally to work well as a liquid desiccant for dehumidifying air in air conditioning applications (Salazar *et al.*, 2018).

During electrospray, there is deformation of a liquid into Taylor cone in a strong electric field, trailed by jet or spray electro-hydrodynamically, (Guo *et al.*, 2019). Research has shown that a steady-state Taylor cone can be identified with full-dimensional simulation based on the Navier-Stokes equation and the Melcher-Taylor leaky dielectric model with the incorporation of VOF to track the dynamic liquid–gas interface, (Wu, et al, 2012).

In this work, CFD simulations in ANSYS FLUENT are presented. A numerical code is developed to simultaneously solve the coupled electrohydrodynamic and electrostatic equations and determine the shape of the liquid at the outlet of the nozzle as an effect of external electric field for a glycerol electrospray in an air dehumidification system. Some assumptions are made, (Rahmanpour,et al, 2017):

i. Density and surface tension are assumed to be uniform and constant.
ii. The electric permittivity of liquid, ε, is constant (isotropic fluid).
iii. The electric conductivity and permittivity of the liquid, k and ε, are such that the so-called electric relaxation time of the charges $t_e \sim k_\varepsilon$ is very small compared to the characteristic break-up time t_b; this condition demands a liquid with sufficient electrical conductivity

During this study, the model will not include a droplet break-up and the dynamics of droplet evaporation, (Najjaran *et al.*, 2013).

2. Governing Equations

Obtaining a solution for the electrohydrodynamic flow equations using CFD can be regarded as a balance amid electrostatic forces and hydrodynamic (Wu, Oleschuk and Cann, 2012). The numerical simulation looks at corona discharge, gas flow, particle charging and transport therefore numerical analysis focused on the electric field, fluid dynamics, particle trajectory, and particle charging (Dong et al., 2019).

In this work the simulations are anchored on Taylor and Melcher leaky dielectric model (LDM) and Navier-Stokes equations (Zeng, et al, no date). Glycerol allows free charge to exist at the liquid-gas interface and jet formation comes by as a result of shear forces at the interface. The surface tension balances the normal electric stress whilst the tangential electric field is balanced by viscous flow, (Wu, et al, 2012).

2.1 Fluid Flow

The simulations involves multiphase flow with the emitter being the solid, air is gas and desiccant is in liquid phase. There is need to simulate the flow so as to obtain the velocity field for velocity profile extraction at devices outlets. The simulation of flow is based on continuity relationships and conservation laws. Wu, et al, (2012) and Gałeka and Strzelczyk, (2019) agree that if the liquid is to be Newtonian, with laminar flow, constant density and viscosity, the continuity of flow velocity becomes :

$\nabla.\vec{v} = 0$…………………………1

where v is flow velocity, and **∇** is the divergence and this equation highlights that there is continuous fluid flow since the expansion rate of volume is zero.
According to Gałek and Strzelczyk, (2019) and Wu, et al, (2012), Navier–Stokes equation for electrohydrodynamic flow is:

$$\rho\frac{d\vec{v}}{dt} = -\nabla P + \eta\nabla v^2 + \vec{f}_c + \rho\vec{g}$$

Where P is the pressure, $\vec{f_c}$is the electromechanical force, η is the viscosity coefficient, and g is the gravitational constant. Fluid acceleration is presented by the left side of the equation whilst right side sums up including pressure gradient, viscous force, shear force and gravitational forces.
To obtain the electromechanical force, $\vec{f_c}$, the space charge density and electric potential are needed. The force is the difference between expected Colulomb force and polarization stress which act at the air-liquid interface, thus it is given by:

$$\vec{f_c} = q\vec{E} - \frac{1}{2}\vec{E}.\vec{E}\nabla_{\varepsilon}$$

Where $\vec{E}$ is the electric field, ε is fluid permittivity and q is the net free charge density near the interface.

2.2 Electric Field

Bulk free charge density is considered negligible with an irrotational and divergence-free electric field with the Laplace equation governing Leaky Dielectric Model. For the electric field in the bulk fluid region, the equation is:

$$\boldsymbol{\nabla}^2\emptyset = 0$$

Where $\emptyset$ is the potential, then the charge conservation law is:

$$\frac{dq}{dt} = -\vec{n}.\sigma(\boldsymbol{\nabla}\emptyset)$$

Where d/dt is Lagrangian derivative, σ is liquid's electrical conductivity whilst $\vec{n}$ denotes the direction normal to the interface.
There is formation of electric field discontinuity in the direction normal to the interface due to the existence of interfacial charge density yet there is need to conserve tangential current thus the equations become:

$$\vec{n}(\varepsilon_1\nabla\emptyset_1\text{-}\varepsilon_m\nabla\emptyset_m) = q$$

$$\vec{t}(\varepsilon_1\nabla\emptyset_1\text{-}\varepsilon_m\nabla\emptyset_m) = 0$$

2.3 Tracking of air–liquid interface using VOF

In FLOW-3D, the Volume of Fluid (VOF) is used to track the moving air–fluid interface whereby a fraction *F* for each cell is introduced. The share of the cell occupied by liquid is given by:

$$F(x,y,t) = \begin{cases} 0 \; outside \; the \; liquid \\ 1 \; inside \; the \; liquid \\ > 0, < 1 \;\; on \; the \; free \; surface \end{cases}$$

And *F* should fulfill the kinematic equation for fluid dynamics:

$$\frac{dF}{dt} + \overrightarrow{v.\nabla F}$$

2.4 Spray current

There is transportation of charges at the base of the Taylor cone due to the conduction to the liquid–air interface. There will be convective flow caused by electric stress's drive of charges at the cone's apex and surrounding liquid. This current conduction and convection currents Icond and Iconv:

$$I = I_{cond} + I_{conv} = \pi R_S^2\vec{E}_z\sigma + 2\pi R_s\vec{u}_z q$$

Where R_s is the jet radius, $\vec{E}_z$is the Z-component of electric filed, $\vec{u}_z$ is axial velocity of jet, q is charge density

3. Numerical Strategy

The equations are solved for a geometry of an emitter which is distance, H, in the range 15–20cm from the collector to ensure compactness of the system. A high potential is then applied between emitter and the extractor with a fluid flow rate of 5ml/hr. The spraying solution is glycerol ($C_3H_8O_3$) with these properties: density=1.261gcm^{-3}, viscosity= 1.412cP (at 25°C), surface tension =63.4mN/m, electrical conductivity =0.05µS/cm, (Salazar *et al.*, 2018). These parameters will be unchanged in the simulations.

The physics preference adopted is CFD with Fluent as the solver. Ansys Fluid Flow (Fluent) DesignerModeler was used to generate an axis-symmetric geometry. The emitter was modeled as infinitely thin cylindrical walls to give high potential gradients in the computation for both cone and jet formation.

For better accuracy during numerical modeling, grid points after meshing should be fine near the nozzle since there will be larger electric potential gradients and be coarse for areas afar. This will ensure accuracy with minimal computational effort since coarseness decreases accuracy whilst fineness increases time. A Cartesian mesh is applied to achieve this, (Rahmanpour, et al 2017).

A multiphase, Volume of Fluid model with 2 phases is used. A pressure based solver with an absolute velocity formula is considered with implicit formulation for volume of fractions parameters and a sharp interface modelling with interfacial anti-diffusion. The phase interactions with surface tension tension force modelling and wall adhesion as adhesion option are considered with a constant coefficient (n/m). The geometry that was modeled in this work is presented in Figure 3.

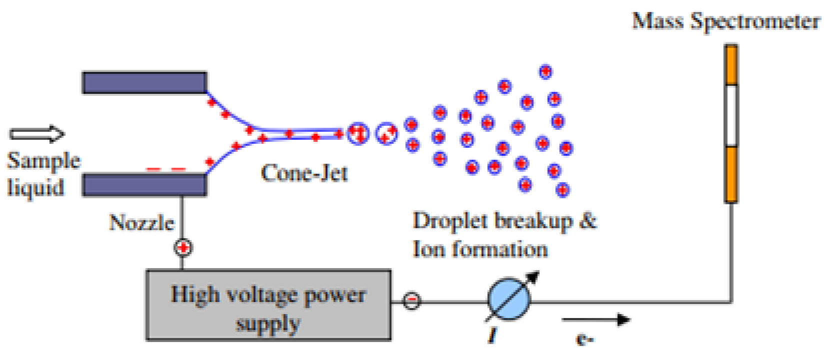

Figure 3: Electrospray configuration

4. Boundary conditions

In order to solve equations discussed in previous sections, boundary conditions should be defined. These conditions are vital at the on the outside of the computational region and at the emitter–fluid interface. A velocity specification method is used which is normal to the boundary. After the fluid pass the zero-voltage plane, there is no acceleration nor deceleration thus there will be a constant velocity. A stationary wall is assumed with a no-slip shear condition, (Rahmanpour, et al 2017). Represented with a Cartesian mesh, symmetric boundary conditions are introduced, which act like a mirror inhibiting fluid and heat flow across the boundary plane. For a multiplexer, the conditions are similar to single-aperture Cartesian case but the interior planes will be symmetric whilst the peripheral ones will be outflow, (Wu, et al 2012; Rahmanpour, et al, 2017).

The solver used was a Presto, a pressure-velocity one, coupled with volume fractions which has a spatial discretization with a Green-Gauss cell based gradient. For the transient formulation, a bounded second order implicit scheme with a second order upwind momentum with hybridization to improve accuracy was used together with compressive volume fraction for fluid flow and free surface,(Wu, et al 2012; Najjaran *et al.*, 2013; Rahmanpour, et al, 2017). The electrical potential is first order upwind.

A variable time step method and standard initialization is employed with a reference frame relative to the cell zone. The solution is found by obtaining the electrical potential first in the computational domain then the electric body force is computed. This force is then fed into the Navier-Stokes eqution which, due to the presence of electric body forces, when solved the liquid is deformed into a jet, (Rahmanpour and Ebrahimi, 2015). Flow field is solved too for the air surrounding, (Figure 4).

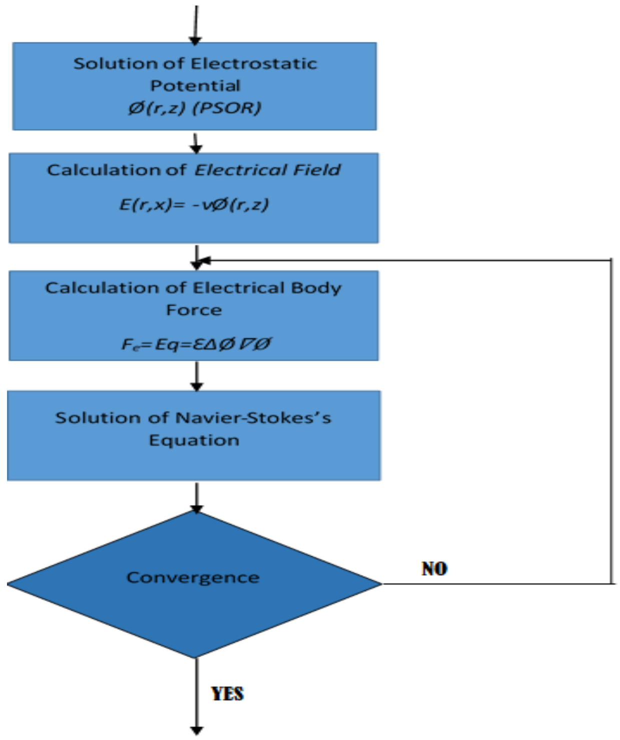

Figure 4: Flow chart for computations

5. Results and Discussions

Emitter design define the surrounding electric field thereby considerably affecting Taylor cone formation, and an example of successful generation of a Taylor cone (Rahmanpour, Ebrahimi and Pourrajabian, 2017) is as presented in Figure 5.

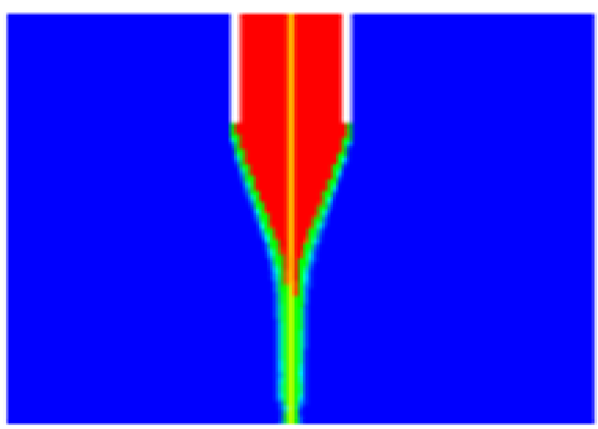

Figure 5: Taylor cone jet for heptane liquid

A constant electric potential difference is applied between the conducting emitter with length L, and a metallic plate, which is at a distance H. Figure 6 shows the numerical simulation result for the generated jet as a result of the applied electric potential at constant voltage and flow rate.

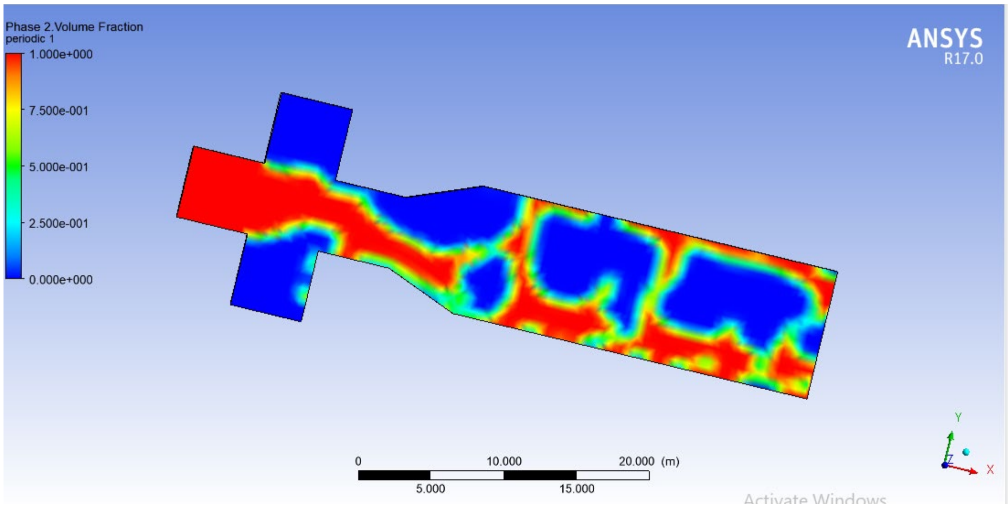

Figure 6: Jet formation

This simulation show that diameter of resulting jet of electrosprayed glycerol quickly disintegrates after the throttle. There is need to simulate jet formation using different emitter diameters in order to come up with a nozzle diameter which results in a strong jet. Varying the electric potential may also help positive results. The volume fraction for jet formation is presented in Figure 7 and it can be seen that glycerol bubbles are generated throughout the time of analysis.

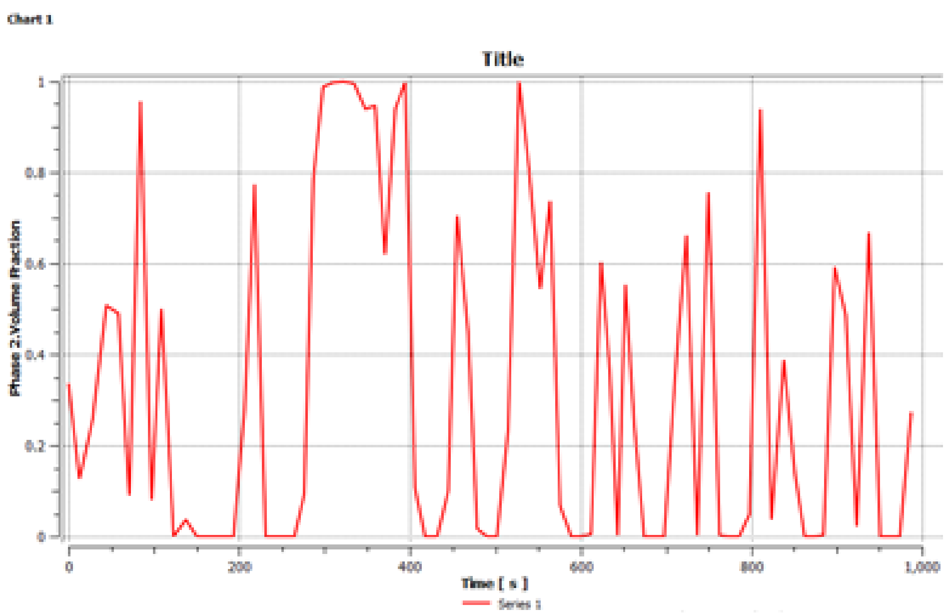

Figure 7: Volume fraction chart

In order to produce a strong jet, it requires a higher onset potential for a liquid with higher surface tension. Contrary to this, an emitter of smaller diameter have need of lower onset potential if the value of surface tension is to be constant. This is for the reason thatreduction in emitter diameter results in a rise in electric field strength. Therefore for better analysis, multi-micro sized emitters are a necessity for quality electrospraying process.

6. Conclusion

In conclusion, Computational Fluid Dynamics simulations in ANSYS FLUENT has been successfully done for glycerol based electrospray. A numerical code has developed to simultaneously solve the coupled electrohydrodynamic and electrostatic equations and determine the shape of cone jet as an effect of the applied electric field in an air dehumidification system. The emitter is observed to have been able to generate a jet with an applied electric potential and given liquid desiccant properties, making it appropriate for the analysis. There is a correlation which exists between spray current and jet diameter and the flow rate, potential difference, surface tension and the viscosity, as confirmed by results in literature.

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