



# **MODELING AND SIMULATION OF TAYLOR CONE AND JETTING FROM LIQUID DROPLETS**

By

Asmaa Mohammed Elkady

A thesis submitted to the

Faculty of Engineering at Cairo University

In partial Fulfillment of

MASTER OF SCIENCE

In

Chemical Engineering

FACULTY OF ENGINEERING, CAIRO UNIVERSITY

GIZA, EGYPT

2016

# **MODELING AND SIMULATION OF TAYLOR CONE AND JETTING FROM LIQUID DROPLETS**

By

Asmaa Mohammed Elkady

A thesis submitted to the

Faculty of Engineering at Cairo University

In partial Fulfillment of

**MASTER OF SCIENCE**

In

Chemical Engineering

Under the supervision of

Prof. Dr. Mai M. Fouad

Prof. Dr. Tarek M. Mostafa

Professor of Chemical Engineering  
Department of Chemical Engineering  
Faculty of Engineering, Cairo university

Professor of Chemical Engineering  
Department of Chemical Engineering  
Faculty of Engineering, Cairo university

Dr. Ahmed S. Eissa

Associate professor of Chemical Engineering  
Department of Chemical Engineering  
Faculty of Engineering, Cairo University

**FACULTY OF ENGINEERING, CAIRO UNIVERSITY  
GIZA, EGYPT  
2016**

# **MODELING AND SIMULATION OF TAYLOR CONE AND JETTING FROM LIQUID DROPLETS**

By

Asmaa Mohammed Elkady Ibrahim

A thesis submitted to the  
Faculty of Engineering at Cairo University  
In partial Fulfillment of  
MASTER OF SCIENCE  
In  
CHEMICAL ENGINEERING

Approved by the  
Examining Committee

---

**Prof. Dr.** Mai M. Kamal El Din, Thesis main advisor

---

**Prof. Dr.** Salwa R. Mostafa, Internal examiner

---

**Prof. Dr.** Hammam Abdel Rahman El-Abd , External Examiner

– Professor of Chemical Engineering, Pilot Plant Department, National  
Research Center.

FACULTY OF ENGINEERING, CAIRO UNIVERSITY  
GIZA, EGYPT  
2016

**Engineer:** Asmaa Mohammed Elkady Ibrahim  
**Date of Birth :** 5 / 4 / 1986  
**Nationality :** Egyptian  
**E-mail :** asmaaelkady@hotmail.com  
**Phone. :** 01224561550  
**Address :** 10, Rasmy from Ahmed badawy st., Shoubra, Cairo, Egypt  
**Registration Date :** 1 / 10 / 2010  
**Awarding Date :** / /  
**Degree :** Master of Science  
**Department :** Chemical Engineering Department



**Supervisors :** **Prof. Dr.** Mai Mohamed Kamal El Din  
**Prof. Dr.** Tarek Mohamed Mostafa  
**Dr.** Ahmed Sherif Eissa

**Examiners :** **Prof. Dr.** Mai Mohamed Kamal El Din (Thesis main advisor)  
**Prof. Dr.** Salwa Raafat Mostafa (Internal examiner)  
**Prof. Dr.** Hammam Abdel Rahman El-Abd (External examiner)

– Professor of Chemical Engineering, Pilot Plant Department, National Research Center.

**Title of Thesis :**  
MODELING AND SIMULATION OF TAYLOR CONE AND JETTING  
FROM LIQUID DROPLETS

**Key Words:**  
Taylor cone; liquid droplet; Electrospinning; momentum balance; applied voltage

**Summary :**  
Liquid droplets are deformed when subjected to an electric field and acquires stable shapes. These shapes are a result of force balance between surface tension force, viscous force and electrostatic force. The droplet shape is turned into a conical shape, which is well known by “Taylor cone” with a half angle of  $49.3^\circ$ ; then a fine jet comes from the cone apex. This phenomenon is widely studied and is strongly related to the electrospinning process which is recognized as an efficient technique to produce nanofibers. Variety of materials is used for electrospinning; most of them are polymers, composites, semiconductors or ceramics. Most of electrospinning experiments were done in research laboratories. The main objective of the research is to simulate the Taylor cone formation and jetting process as a part of electrospinning process using COMSOL® Multiphysics program. Three materials are used in this simulation; glycerol, distilled water and NaCl solution.



## **Acknowledgements**

First and foremost, I would like to express my profound gratitude, and thanks to my supervisor, Dr. Ahmed S. Eissa for his continuous support, invaluable advice, and constant guidance throughout the duration of this work. I would also like to thank Prof. Tarek M. Mostafa for his valuable suggestions and constructive comments that were very beneficial in my completion of this work. In particular, I would like to give a special thanks to Prof. Mai M. Fouad for her great support and kind help.

I also wish to express my appreciation to my M.Sc. committee (Prof. Hammam A. El-Abd and Prof. Salwa R. Mostafa) for their valuable comments.

Finally, my deepest gratitude goes to all the members of my family and to my friends for their life- long love, care and support.

## **Dedication**

I dedicate this thesis to my great mother

You have successfully made me the person I am becoming

This work is also dedicated to my husband, Ashraf

I am truly thankful for having you in my life

# Table of Contents

<b>ACKNOWLEDGMENTS.....</b>	<b>I</b>
<b>DEDICATION.....</b>	<b>II</b>
<b>TABLE OF CONTENTS.....</b>	<b>III</b>
<b>LIST OF TABLES.....</b>	<b>VI</b>
<b>LIST OF FIGURES.....</b>	<b>VII</b>
<b>ABSTRACT.....</b>	<b>X</b>
<b>CHAPTER 1: INTRODUCTION.....</b>	<b>1</b>
1.1 Introduction.....	1
1.2 Apparatus.....	3
1.3 Controlling parameters.....	5
1.3.1 Physical properties of jetted liquid.....	5
1.3.1.1 Surface tension.....	5
1.3.1.2 Viscosity.....	5
1.3.1.3 Electrical conductivity.....	5
1.3.1.4 Relative permittivity.....	5
1.3.2 Processing conditions.....	6
1.3.2.1 The applied voltage.....	6
1.3.2.2 Distance between needle tip and grounded plate.....	7
1.3.2.3 Needle diameter.....	7
1.3.2.4 Flow rate.....	8
1.4 Research objectives.....	8
<b>CHAPTER 2: LITERATURE REVIEW.....</b>	<b>9</b>
2.1 Introduction.....	9
2.2 Related works.....	9
<b>CHAPTER 3: THEORETICAL STUDY.....</b>	<b>11</b>
3.1 Introduction.....	11
3.2 Governing equations.....	11
3.2.1 The equation of continuity.....	11
3.2.2 Navier-Stokes equation.....	11
3.2.3 Gauss' law for electric field.....	12
3.2.3.1 Electrostatics.....	12
<b>CHAPTER 4: MODELING AND SIMULATION.....</b>	<b>15</b>

4.1 Introduction.....	15
4.2 Model definition.....	15
4.3 Material properties and processing conditions.....	16
4.3.1 Glycerol model.....	16
4.3.2 Distilled water model.....	16
4.3.3 NaCl solution model.....	17
4.4 Simulation on COMSOL Multiphysics®.....	17
4.4.1 Introduction to level set method.....	18
4.4.2 Level set function.....	18
4.4.3 Laminar two phase flow, level set interface.....	20
4.4.4 Electrostatic interface.....	21
4.4.5 Coupling the two interfaces.....	21
4.4.6 Relative permittivity equation.....	22
4.5 Initial and boundary conditions.....	22
4.6 Selecting mesh.....	22
<b>CHAPTER 5: RESULTS .....</b>	<b>24</b>
5.1 Effect of droplet shape on Taylor cone half angle.....	24
5.1.1 Droplet dimensions.....	24
5.1.2 Effect of initial droplet shape on modeling glycerol.....	27
5.1.3 Effect of initial droplet shape on modeling distilled water.....	30
5.1.4 Effect of initial droplet shape on modeling NaCl solution.....	34
5.2 Effect of applied voltage variation on half angle $\theta$ .....	37
5.2.1 Effect of voltage applied on $\theta$ of glycerol.....	38
5.2.2 Effect of voltage applied on $\theta$ of distilled water.....	41
5.2.3 Effect of voltage applied on $\theta$ of NaCl solution.....	44
5.3 Effect of interface thickness on Taylor cone half angle $\theta$ .....	48
5.3.1 Effect of interface thickness on Taylor cone half angle of glycerol.....	50
5.3.2 Effect of interface thickness on Taylor cone half angle of distilled water.....	50
5.3.3 Effect of interface thickness on Taylor cone half angle of NaCl solution.....	51
5.4 Effect of needle diameter on Taylor cone half angle.....	52
5.4.1 Effect of needle diameter on $\theta$ for glycerol.....	53
5.4.2 Effect of needle diameter on $\theta$ for distilled water.....	55
5.4.3 Effect of needle diameter on $\theta$ for NaCl solution.....	58
<b>CHAPTER 6: DISCUSSION AND CONCLUSIONS.....</b>	<b>61</b>
6.1 Initial droplet shape, shear stress and Taylor cone half angle.....	61
6.2 Electric potential and electric force components.....	66
6.3 Electric potential distribution and electrode polarity.....	69
6.4 Surface tension force and surface tension coefficient.....	72

6.5 Conclusions.....	74
<b>REFERENCES.....</b>	<b>76</b>

## List of tables

<b>Table (5.1):</b> Dimensions of initial droplet.....	24
<b>Table (5.2):</b> Taylor cone half angle with different needle diameters for glycerol model.....	53
<b>Table (5.3):</b> Taylor cone half angle with different needle diameters for distilled water model.....	55
<b>Table (5.4):</b> Taylor cone half angle with different needle diameters for NaCl solution model.....	58
<b>Table (6.1):</b> Surface tension force along the interface for glycerol droplets attached to different needle diameters.....	73
<b>Table (6.2):</b> Surface tension force along the interface for distilled water droplets attached to different needle diameters.....	73
<b>Table (6.3):</b> Surface tension force along the interface for NaCl solution droplets attached to different needle diameters.....	73

## List of figures

<b>Figure (1.1):</b> Droplet deformation progress during electrospinning, (a) Taylor cone, (b) Single jet emanates from the tip of Taylor cone, (c) Bending instability.....	2
<b>Figure (1.2):</b> Taylor cone instability and emanating of a high density charged jet.....	2
<b>Figure (1.3):</b> Potential applications of electrospun nanofibres.....	3
<b>Figure (1.4):</b> Apparatus used to perform electrospinning experiments.....	4
<b>Figure (3.1):</b> Equations relating the three fundamental quantities of electrostatics.....	13
<b>Figure (4.1):</b> 2D axis symmetry schematic applied in the three models.....	16
<b>Figure (4.2):</b> Dielectric constant of distilled water after NaCl addition at various temperatures.....	17
<b>Figure (4.3):</b> Forces balance on Taylor cone.....	18
<b>Figure (4.4):</b> Free triangle mesh distribution.....	23
<b>Figure (5.1):</b> 2D axisymmetrical initial droplet shape (a) droplet I, (b) droplet II, (c) droplet III.....	25
<b>Figure (5.2):</b> 3D initial droplet shape; (a) droplet I, (b) droplet II, (c) droplet III.....	27
<b>Figure (5.3):</b> Glycerol droplet I; (a) 3D Taylor cone at $t = 20$ ms, (b) Taylor cone half angle $\theta = 39.52^\circ$ .....	28
<b>Figure (5.4):</b> Glycerol droplet II, (a) 3DTaylor cone at $t = 31$ ms, (b) Taylor cone half angle $\theta = 40.54^\circ$ .....	29
<b>Figure (5.5):</b> Glycerol droplet III, (a) 3D Taylor cone at $t = 15$ ms, (b) Taylor cone half angle $\theta = 49.88^\circ$ .....	30
<b>Figure (5.6):</b> Distilled water droplet I, (a) 3D Taylor cone formation at $t = 1.21$ ms, (b) Taylor cone half angle $\theta = 39.79^\circ$ .....	32
<b>Figure (5.7):</b> Distilled water droplet II, (a) Taylor cone formation at $t = 0.7$ ms, (b) Taylor cone half angle $\theta = 41.81^\circ$ .....	33
<b>Figure (5.8):</b> Distilled water droplet III, (a) 3D Taylor cone formation at $t = 0.9$ ms, (b) Taylor cone half angle $\theta = 51.05^\circ$ .....	34
<b>Figure (5.9):</b> NaCl solution; droplet I, (a) 3DTaylor cone formation at $t = 1$ ms, (d) 2D Taylor cone half angle $\theta = 40.6^\circ$ .....	35
<b>Figure (5.10):</b> NaCl solution droplet II, (a) 3D Taylor cone formation at $t = 1$ ms, (b) Taylor cone half angle $\theta = 45.04^\circ$ .....	36

<b>Figure (5.11):</b> Taylor cone for NaCl solution; droplet III, (a) 3D Taylor cone formation at $t = 1.07$ ms, (b) Taylor cone half angle $\theta = 50.5^\circ$ .....	37
<b>Figure (5.12):</b> Volume fraction of glycerol droplet when $V = 0$ at times 0, 20, 40, 60, 80, 100 ms.....	39
<b>Figure (5.13):</b> Volume fraction of glycerol, (a) $V = 0$ , $t = 100$ ms, (b) $V = 5$ kV, $t = 100$ ms, (c) $V = 7$ kV, $t = 100$ ms, (d) $V = 9$ kV, $t = 80$ ms, (e) $V = 10$ kV, $t = 65$ ms, (f) $V = 11$ kV, $t = 25$ ms.....	40
<b>Figure (5.14):</b> Glycerol jet from Taylor experiment, the critical voltage according to Taylor experiments are ranging from 9.5 kV to 17.5 kV.....	41
<b>Figure (5.15):</b> Volume fraction of distilled water at times 0, 1, 2, 3, 4, 5 ms.....	42
<b>Figure (5.16):</b> Volume fraction of distilled water, (a) $V = 0$ , $t = 5$ ms. (b) $V = 3$ kV, $t = 5$ ms, (c) $V = 4$ kV, $t = 3.5$ ms (d) $V = 5$ kV, $t = 3$ ms, (e) $V = 6$ kV, $t = 2.5$ ms, (f) $V = 7$ kV, $t = 2$ ms.....	44
<b>Figure (5.17):</b> Taylor experimental results for distilled water (a) $V = 0$ , (b) $V = 3$ kV, (c) $V = 7.8$ kV, (d) $V = 4$ kV.....	44
<b>Figure (5.19):</b> Volume fraction of distilled water at times 0, 1, 2, 3, 4, 5 ms.....	46
<b>Figure (5.20):</b> Volume fraction of NaCl solution, (a) $V = 0$ kV, $t = 5$ ms, (b) $V = 3$ kV, $t = 5$ ms, (c) $V = 4$ kV, $t = 5$ ms, (d) $V = 5$ kV, $t = 3$ ms, (e) $V = 11$ kV, $t = 1.6$ ms, (f) $V = 12$ kV, $t = 1.5$ ms.....	47
<b>Figure (5.21):</b> Taylor experimental results for NaCl solution jet (a) $V = 0$ kV, (b) $V = 10$ kV, (c) $V = 12$ kV.....	48
<b>Figure (5.22):</b> Geometry discretization with different mesh size. (a) Normal mesh, (b) Fine mesh, (c) Finer mesh, (d) Extra fine mesh, (e) extremely fine mesh.....	49
<b>Figure (5.23):</b> Glycerol droplet progress using different interfaces thickness (a) $\varepsilon = 0.0106$ cm, $\theta \approx 44.2^\circ$ , (b) $\varepsilon = 0.0074$ cm, $\theta \approx 43.01^\circ$ , (c) $\varepsilon = 0.004$ cm, $\theta \approx 49.88^\circ$ , (d) $\varepsilon = 0.002$ cm, $\theta \approx 49.88^\circ$ .....	50
<b>Figure (5.24):</b> Taylor cone formation for distilled water, (a) $\varepsilon = 0.0106$ cm, $\theta \approx 35.27^\circ$ , (b) $\varepsilon = 0.0074$ , $\theta \approx 35.27^\circ$ , (c) $\varepsilon = 0.004$ cm, $\theta \approx 41.8^\circ$ , (d) $\varepsilon = 0.002$ cm and $\theta \approx 51.05^\circ$ .....	51
<b>Figure (5.25):</b> Taylor cone formation for NaCl solution, (a) $\varepsilon = 0.0106$ cm, $\theta \approx 33.06^\circ$ , (b) $\varepsilon = 0.0074$ , $\theta \approx 35.7^\circ$ , (c) $\varepsilon = 0.004$ cm, $\theta \approx 46.3^\circ$ , (d) $\varepsilon = 0.002$ cm and $\theta \approx 33.06^\circ$ .....	52
<b>Figure (5.26):</b> Taylor cone formation and jetting glycerol in different needle diameters; (a) $r = 0.5$ mm, (b) $r = 0.6$ mm, (c) $r = 0.7$ mm, (d) $r = 0.8$ mm, (e) $r = 0.9$ mm, (e) $r = 0.1$ mm.....	55

<b>Figure (5.27):</b> Taylor cone formation and jetting distilled water in different needle diameters; (a) $r = 0.5\text{mm}$ , (b) $r = 0.6\text{mm}$ , (c) $r = 0.7\text{mm}$ , (d) $r = 0.8\text{mm}$ , (e) $r = 0.9\text{mm}$ , (e) $r = 0.1\text{ mm}$ .....	58
<b>Figure (5.28):</b> Taylor cone formation and jetting NaCl solution in different needle diameters; (a) $r = 0.5\text{ mm}$ , (b) $r = 0.6\text{ mm}$ , (c) $r = 0.7\text{mm}$ , (d) $r = 0.8\text{mm}$ , (e) $r = 0.9\text{mm}$ , (e) $r = 0.1\text{ mm}$ .....	60
<b>Figure (6.1):</b> Shear stress values acting on glycerol droplets. (a) glycerol droplet I, (b) glycerol droplet II, (c) glycerol droplet III.....	63
<b>Figure (6.2):</b> Shear stress values acting on distilled water droplets. (a) droplet I, (b) droplet II, (c) droplet III.....	64
<b>Figure (6.3):</b> Shear stress values acting on NaCl solution droplets. (a) droplet I, (b) droplet II, (c) droplet III.....	66
<b>Figure (6.4):</b> Electrical force components ( $F_r$ , $F_z$ ) acting on glycerol for different values of applied voltages.....	67
<b>Figure (6.5):</b> Electrical force components ( $F_r$ , $F_z$ ) acting on distilled water for different values of applied voltages.....	68
<b>Figure (6.6):</b> Electrical force components ( $F_r$ , $F_z$ ) acting on NaCl solution for different values of applied voltages .....	69
<b>Figure (6.7):</b> Snapshots of Glycerol interface with increments of 20 ms from top to bottom. Left: $V = 11\text{ kV}$ , right: $V = -11\text{ kV}$ .....	70
<b>Figure (6.8):</b> Snapshots of distilled water interface with increments of 2 ms from top to bottom. Left: $V = 7\text{ kV}$ , right: $V = -7\text{ kV}$ .....	71
<b>Figure (6.9):</b> Snapshots of NaCl solution interface with increments of 2 ms from top to bottom. Left: $V = 12\text{ kV}$ , right: $V = -12\text{ kV}$ .....	72

## Abstract

Liquid droplets are deformed when subjected to an electric field and acquires stable shapes. These shapes are a result of force balance between surface tension force, viscous force and electrostatic force. This occurs when liquid droplet is held at a capillary tube by its surface tension, this capillary tube is raised to high potential and a grounded plate is placed in an appropriate distance from the capillary. The droplet remains stable until the potential difference between the droplet and the plate exceeds the critical value. If the electric potential is raised above this critical value the droplet shape is turned into a conical shape. This conical shape is well known by “Taylor cone” with a half angle of  $49.3^\circ$ ; then a fine jet comes from the cone apex. This phenomenon is widely studied and is strongly related to the electrospinning process which is recognized as an efficient technique to produce nanofibers.

Electrospinning process involves two stages. During the first stage, at which the Taylor cone forms, the jet emerges from the needle tip and steadily stretches downstream by electrostatic forces. In the second stage, the polymer jet becomes sufficiently thin and bending instability occurs, then the thinned fiber spirals violently. Variety of materials is used for electrospinning; most of them are polymers, composites, semiconductors or ceramics. Most of electrospinning experiments were done in research laboratories. Many studies, theories and experiments were done in order to have a clear explanation for the first stage in electrospinning process. For this stage, Hohman et.al. presented a slender body theory for electrospinning of Newtonian fluids. Spivak and Dzenis introduced a power law viscosity model. Renker et. al. modeled the viscoelasticity of the jet by a linear Maxwell equation. The first stage of electrospinning process is important because cone formation and jetting are the basis for the analysis of the second stage of jet instability. Also first stage sets up the conditions for the second stage of electrospinning process.

Electrospinning is a complex process to be studied. This complexity is due to the coupling of electrostatic forces and momentum forces. Although electrospinning process is a century old technology and an important subject for recent intensive researches, there is no clear understanding of the behavior of the electrospun jet and parameters affecting the whole process. Moreover, the results gathered from experimental researches contain significant inconsistencies. Very little researches examined the effect of electrical parameters on the electrospun jet, such as the polarity of electrode, fluid conductivity and fluid permittivity. Furthermore, no researches were concerned with optimization of the electrospinning process. So, a comprehensive investigation is needed for optimization of electrospinning process and finds the favorable parameters and conditions for this process. The cone- Jet models become in the forefront of 1990's researches that are concerned with droplets dynamics with the rapid development of Nano technology in either experimental researches or theoretical studies. Theoretical studies are limited to gross simplification of the actual problem because of the complication which accompanied the analysis of the coupled fluid