AMERICAN UNIVERSITY OF BEIRUT

A MATHEMATICAL MODEL TO PREDICT ELECTRONIC CIGARETTE NICOTINE YIELD

by
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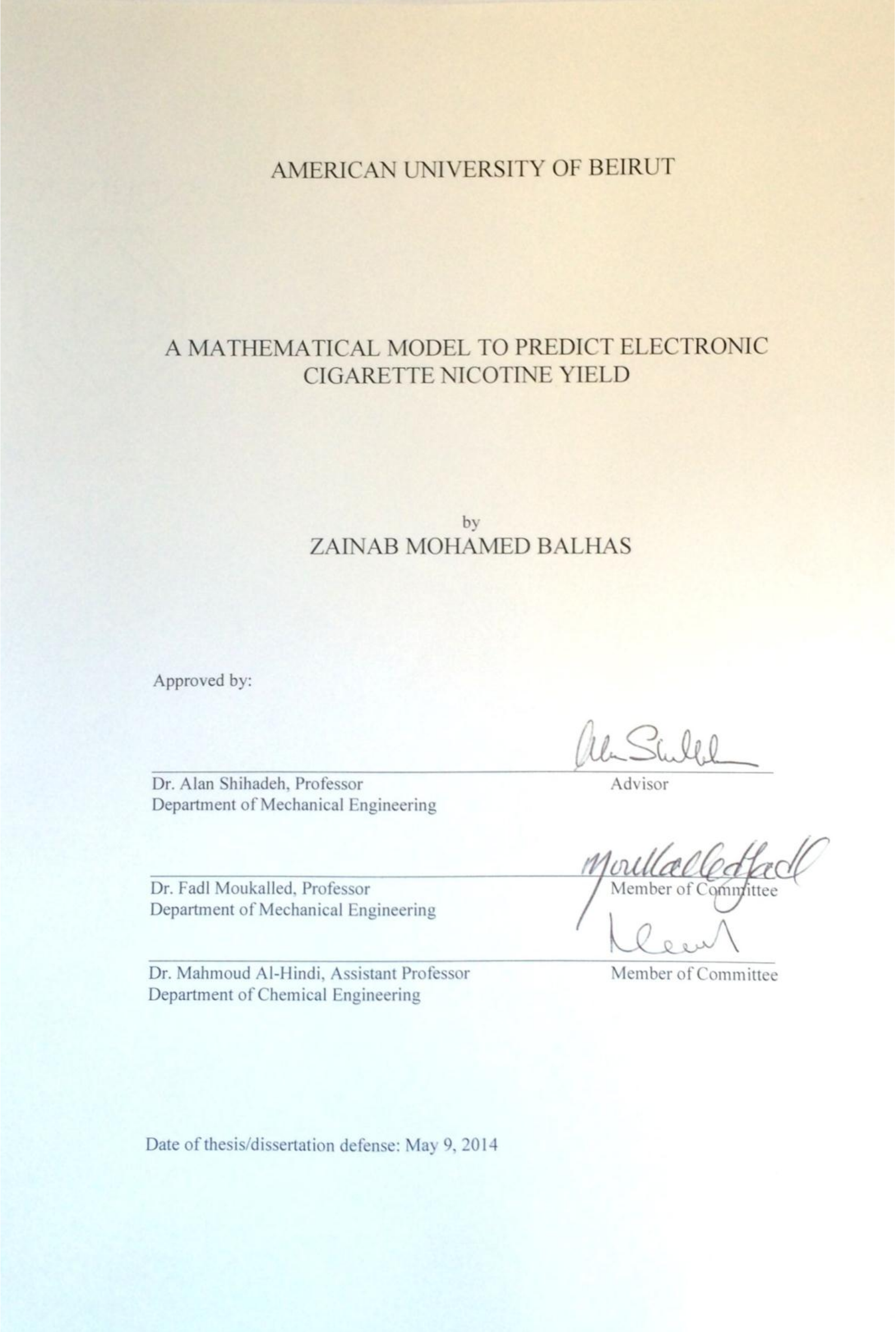

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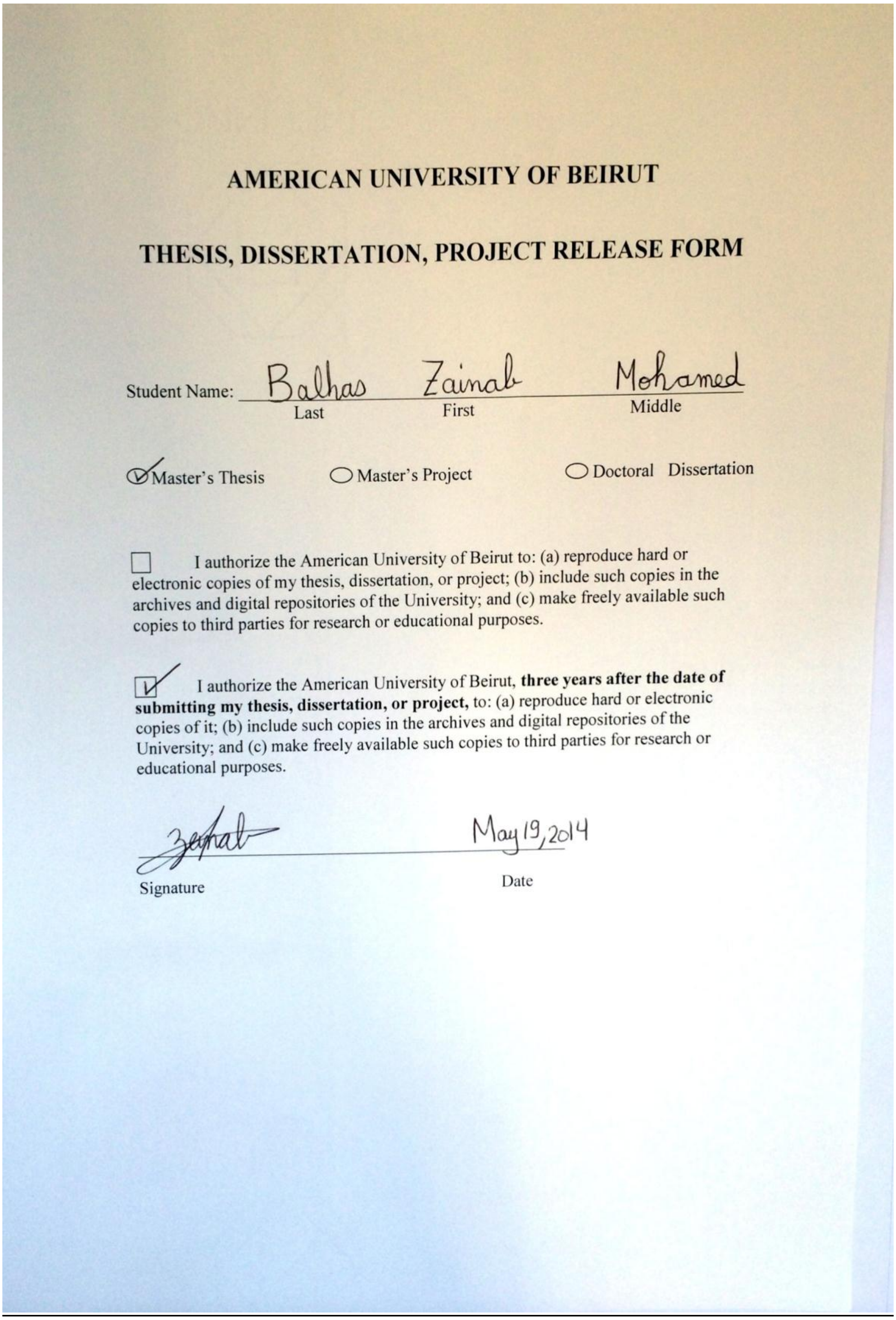

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All thanks to the greatest giver of all good, to God, the most beneficent, the most merciful, as He guides me through life and showers me with His infinite blessings and bounties.

AN ABSTRACT OF THE PROJECT OF

Zainab Mohamed Balhas for Master of Mechanical Engineering
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Title: A Mathematical Model to Predict Electronic Cigarette Nicotine Yield

Electronic cigarettes (ECIGs) are devices designed to deliver nicotine and some sensory features of cigarette smoking without combusting tobacco. They are marketed as a reduced harm smoking alternative to conventional cigarette. While they have become increasingly popular in recent years, little is known about their safety and efficacy. With continuously and rapidly evolving product design features and use behaviors, public health officials face the task of developing regulations for an ever moving target. Though design features and user behavior highly influence ECIG nicotine emission and understanding these factors is relevant to regulation, evaluating these factors in the human or analytical lab is a time consuming and costly process.

In this study, a mathematical model based on principles of heat and mass transfer was developed to help regulators rapidly screen proposed product designs based on nicotine emissions. The model predicts potential nicotine and particulate matter yield from ECIG devices as a function of design features and user puffing behavior. The predicted variables from the model were tested against experimental measurements conducted over a range of ECIG design features and puff variables. The results show that the predicted and measured values are strongly correlated, with high coefficients of determination. The results also revealed that the different factors affecting nicotine emissions were well captured in the mathematical model. Thus, this model can be used to identify products that are likely to be ineffective or to pose increased risk of abuse potential, and to help guide selection of use conditions and product designs for subsequent human laboratory investigations.

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NOMECLATURE

A_{surf}	surface area of the coil (m^2)
C	vapor concentration (kg/m^3)
c_p	specific heat (J/(kg.K))
D	binary diffusion coefficient in air (m^2/s)
d	diameter (m)
dt	time step (sec)
h	enthalpy (J/kg)
h_{fg}	latent heat of vaporization (J/kg)
h_m	mass transfer coefficient (m^2/s)
h_t	heat transfer coefficient (W/(m^2.K))
k	thermal conductivity (W/(m.K))
M	molar mass (kg/mol)
m	mass (kg)
P	pressure (Pa); perimeter (m)
R	electrical resistance of the coil (Ω)
Rt	thermal resistance (K/W)
Ru	universal gas constant (J/(mol.K))
s	shape factor (m)
T	temperature (K)
V	voltage of the power unit (Volts); Volume (m^3)
Y	mole fraction

Greek Letters

σ	Stefan-Boltzmann constant (W/(m^{2}K^4))

Subscripts

a	air
amb	ambient
c	coil
c1	wet coil
c2	dry coil
cer	ceramic
f	fluid
i	inlet
mix	mixture
nic	nicotine
o	outlet
pg	propylene glycol
vg	vegetable glycerin
s	solder
v	vapor

To the lady I was named after, from whom I learned the virtues of bravery and patience,
to the lady of knowledge, Sayida Zainab (A.S.)

CHAPTER I

INTRODUCTION

Electronic nicotine delivery systems, also called electronic cigarettes or e-cigarettes (ECIG), have become increasingly widespread in the past few years, with estimated global sales in 2014 reaching $2 billion and an increasing number of major tobacco companies introducing ECIG product lines[1]. ECIGs are designed to deliver nicotine to users without burning tobacco [2]. Because there is no combustion, ECIGs are expected to deliver far fewer chemical components than do conventional cigarettes [3, 4]. Figure 1 shows the main components of a typical ECIG. It consists mainly of a power unit, heating element, and cartridge that contain nicotine in solution. The solution—also termed as "juice", "liquid" or "e-liquid"—usually contains propylene glycol (PG) and/or vegetable glycerin (VG), nicotine, and flavorings.

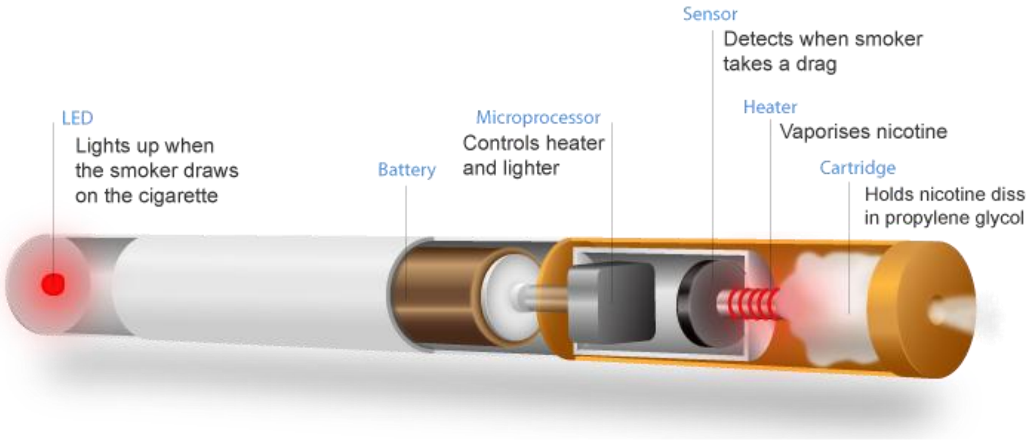

Figure 1.Schematic Diagram of an E-cigarette (http://www.smokelessselects.eu/en/)

When the user sucks air at the mouthpiece, the heating element ("heater coil") is activated (a microcircuit allows electrical current to pass through the heater coil). The coil heats the nicotine containing solution, causing solution to vaporize. The ambient air drawn in via inlet ports transports the vaporized components away from the heating element where the vapor cools and condenses to form an aerosol of liquid particulate matter droplets suspended in predominately air. The aerosol is then drawn out of the mouthpiece and inhaled by the user.

ECIGs are increasingly available and cheap. In many countries they are sold over the Internet and are also commonly available in tobacco stores, pharmacies, supermarkets, and gasoline stations [5]ECIG advertisement has bloomed through Web sites, social networking sites such as Facebook and through numerous YouTube promotional videos [5]. Also, there are abundant Internet forums that guide people on how to use ECIGs. They have also entered the world of Hollywood through popular movies, television shows and as free giveaways to guests at the 2010 Grammy Awards [6]. ECIG marketing strategies are similar to those of conventional tobacco products [5-7].

Tobacco companies are revealing the vital role that ECIGs play in their future business plans. Ruyan Group, Ltd. reported worldwide revenues of approximately $54 million, and Vapor Corp reported $7.95 million in US sales in 2009[5, 8]. On March 2014, a report from Wells Fargo securities puts the estimated total size of the ECIG retail market in the US at $2 billion [1]

ECIGs are advertised as a less harmful alternative to smoking, though insufficient scientific data are available to support such promotion. Some advertising claims include that "cancer causing chemicals found in tobacco cigarettes are not found in electronic cigarettes", and "no first or second hand smoke", and that "its [emissions are] simply water vapor" [9].

ECIGs vary widely in design, contents and operational features, which very likely affect nicotine yield. Most ECIGs resemble traditional cigarettes and simulate the visual, sensory, and behavioral aspects of smoking traditional cigarettes [5]. Their power units come with a wide range of voltages. Some have a fixed voltage and other have adjustable voltage with a range of 3-7 V.

The heating element may be integrated within the mouthpiece section or it may be a distinct piece between the battery and mouthpiece section of the device[4]. In the second case, the user might engage in unorthodox use behaviors. For example the user might directly drip nicotine liquid on the heater [3]. Moreover, there are different nicotine concentrations levels available, ranging from 0 to 36 mg/ml and an almost inexhaustible range of flavors (e.g. tobacco, fruit, menthol, and many others) [10].

Also, people can mix their own liquids. Instructions are available, for example, on YouTube, and online calculators assist do-it-yourself preparation of liquids. When creating their own mixtures, people can use not only substances contained in commercially available refill products, but also all kinds of other substances. For example, in one video a woman mixing her own liquid replaces water by vodka [7].

In addition to the above design features which can be adjusted by the smoker, user behavior including puff duration, inter-puff interval, puff volume, and puff number can also have a major effect on nicotine delivery from the ECIG.

Market proliferation, unproven health claims, and sales of wide ranging design features are facilitated by the fact that ECIGs are almost completely unregulated and untaxed. All the above factors, with the increase in the ECIGs use [11-14] and with the users' belief that ECIGs are less harmful than conventional products [15], highlight the need for developing tools needed to evaluate and regulate this novel, fast-evolving product. Regulation should be based on verifiable and scientific evidence that necessarily involves evaluating the toxicant emissions, including nicotine.

Unfortunately little objective evidence is known about ECIGs safety and effectiveness. However, while the knowledge base is meager, separate investigators working with varied methods have begun to provide information relevant to regulation. This work is reviewed in the sections below, followed by a statement of objectives for this thesis.

Nicotine has many effects on the body. It raises blood pressure and heart rate, curbs appetite, increases basal metabolic rate and activates bowel movements, which may lead to diarrhea [7]. In the brain, nicotine promotes release of several neurotransmitters causing various psychological effects, which may lead to nicotine dependence [7]. One study of experienced ECIG users has found that using a nicotine-containing ECIG resulted in an increase in plasma nicotine levels, along with an increase in heart rate, indicating that at least some ECIG users are receiving physiologically relevant doses of nicotine [7].

From the laboratory studies, it has been found that some ECIGs are capable of delivering nicotine to their users [16] though others may not be [16, 17]. It has also been found that EC brands and models differ in their efficacy and consistency of nicotine vaporization [12]. It was also found that under some use conditions ECIGs could deliver nicotine in an amount similar the maximum allowable nicotine content of one tobacco cigarette [18].

As for the nicotine content in the e-liquid, nicotine traces and other harmful substances have been found in ECIGs labeled as “nicotine-free” [19, 20]. There was also more nicotine in a product labeled as “low nicotine” than that labeled as “medium” [5]. Thus, the nicotine labeling of the product is not always accurate. It has been speculated that incorrect labeling of nicotine content can lead people to nicotine addiction and they might then switch to other tobacco products such as conventional cigarettes [10]

There is a lack of quality control in the manufacturing, marketing, and distribution of ECIGs. In addition to incorrect labeling of nicotine levels in ECIGs, investigators have found incorrect filling of orders, inaccurate instructions and advertisements, and dead batteries in new products [5]. Variations in the chemical composition of the same flavor in different production batches were also reported [7].

Since 2008, the U.S. Food and Drug Administration (FDA) has received 47 reports about side effects of ECIGs. The following are from the severe adverse events included in the reports: pneumonia, congestive heart failure, burns due to explosion of the product, possible infant death secondary to choking on an ECIG cartridge [7]

Few studies have been conducted on the chemical contents of ECIGs and vapor. These studies were for a limited number of products. The little scientific evidence available reveals that toxicants and carcinogens are present in ECIG cartridges and vapor, although in lower concentrations than in regular cigarettes[5, 19, 21, 22]. There are currently no studies available on the effects of long-term use of ECIGs.

ECIGs have been found to suppress tobacco abstinence symptoms partially [23, 24]. They also have potential to reduce concurrent use of tobacco cigarettes [25, 26]. ECIG users are mainly smokers, smokers considering stopping smoking, and former smokers [7]. From the surveys, the main reason for using ECIG is as an alternative to traditional cigarette [7]. Users' perceptions of why ECIG are useful in quitting smoking were summarized by five themes: bio-behavioral feedback, social benefits, hobby elements, personal identity, and distinction between smoking cessation and nicotine cessation [27].

User behavior should be considered when assessing ECIGs effects in laboratory and when developing a standard protocol for evaluating ECIGs performance. However, currently, there is no standard puff topography for ECIG. The few studies that have addressed this question found that ECIGs use topography is significantly different than for cigarette smoking [18]. Puff duration was significantly longer for ECIGs users (mean of 4.3 s) than for conventional cigarette users (mean of 2.4 s) and puff duration varied significantly among ECIGs brands [2].

A. Thesis Objective

As mentioned above, ECIG design features and user behavior are widely varied, and continuously evolving. However, evaluating the wide range of design features under an expansive range of puff behavior in the human or analytical lab is a time consuming and costly process. The aim of this thesis is to develop and empirically validate a mathematical model that can be used to predict ECIG nicotine emissions based on product design features and human puffing behavior. This model will be useful for regulators and scientists to rapidly screen products for safety and efficacy with regard to nicotine. The innovation in this work is the application of mathematical modeling as a potential regulatory tool. As mentioned above, ECIGs vary widely in design features which likely influence nicotine yield, and thus provide a perfect exemplar to use in a demonstration of the value of mathematical modeling. To our knowledge mathematical models have never been used to predict the nicotine associated with a novel tobacco product.

CHAPTER II

THEORY

A. Problem Description and model

When a user draws a puff from the mouthpiece of an ECIG, air is delivered via a transfer tube to the heating element, where nicotine-containing e-liquid is vaporized. The vapor is then mixed with air, which transports the vaporized components away from the hot heater coil to the mouthpiece, where the vapor cools. A portion of the cooled vapor condenses to form an aerosol, which is then inhaled by the user. The remaining portion re-condenses on the internal surfaces of the mouthpiece and therefore the user does not inhale it. From the above description, three main processes are happening in the ECIG: evaporation of e-liquid and nicotine, mixing of the vapor with the drawn air, and condensation of the vapor. These processes are displayed in Figure 2. Since a fraction of the vapors do not exit the mouthpiece, the evaporated quantity of e-liquid at the heater coil represents a theoretical upper limit, or “potential mass” emitted from the ECIG during a given puff or series of puffs.

In this work, the effort is focused on modeling the first two processes to predict the potential mass of nicotine and e-liquid emitted from the vaporizer and to get the temperature of the air-vapor mixture. Hence, the model is divided into two parts representing the evaporation and mixing processes respectively. Each part requires certain inputs to give predicted outputs; these processes will be more elaborated upon in the subsequent sections.

Energy and mass conservation equations are the main equations used in this model in order to compute the evaporated nicotine and e-liquid from ECIG as a function of design features and user behavior. A common ECIG design was used for developing the preliminary model and then the model was adapted to include the key features that differentiate each used design from the other. To understand the design and operational features, we reverse-engineered the ECIG and drew a schematic diagram embodying its parts (Figure 3).

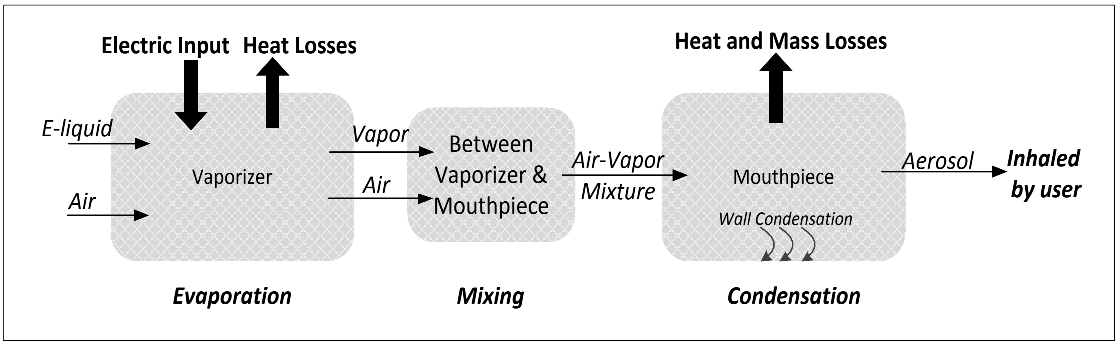

Figure 2.Processes occurring in ECIG

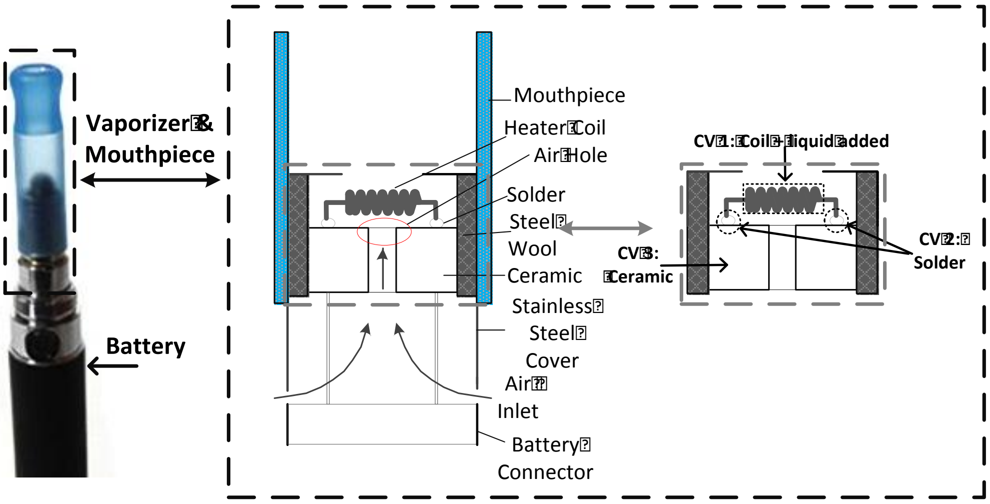

Figure 3.Anatomy of the ECIG

B. Evaporation Model

The vaporizer, where evaporation of e-liquid takes place, is divided into three control volumes. The coil and the e-liquid added to the coil as one control volume. The second control volume is the solder that connects the coil to the internal body of the atomizer. The internal body is the third control volume; it is made from ceramic for this ECIG design. Figure 3 shows the location of the three control volumes.

The coil is modeled as a solid cylinder; the air passing across the coil is considered as a cross flow over a horizontal cylinder. E-liquid is considered as an ideal solution consisting of PG with trace amounts of nicotine where the vapor pressure of the solution obeys Raoult's law, and the activity coefficient of each component (PG and nicotine) is equal to one.

When the coil is totally wet (the coil is completely covered by e-liquid), control volume 1 is taken as one zone (wet zone). However, when the coil starts getting dry (wet-dry), it is taken as two zones (wet and dry) where evaporation of the liquid will happen only in the wet zone.

Taking in consideration the above assumptions, energy and mass conservation equations are given as follows:

Temperature of Coil (Wet Condition)

$$(m_{pg}c_{p_{pg}} + m_c c_{p_c})\frac{dT_c}{dt} = \dot{E} - \dot{Q}_{conv} - 2\dot{Q}_s - \dot{Q}_{rad} - \dot{m}_{pg}h_{fg} \tag{1}$$

Temperature of Coil (Wet-Dry Condition)

$$\left(m_{pg}c_{p_{pg}} + m_c c_{p_c}\right)\frac{dT_{c1}}{dt} = x\dot{E} - x\dot{Q}_{conv} - 2\dot{Q}_s - x\dot{Q}_{rad} - x\dot{m}_{pg}h_{fg} \tag{2}$$

$$(m_c c_{p_c})\frac{dT_{c2}}{dt} = (1-x)\dot{E} - (1-x)\dot{Q}_{conv} - 2\dot{Q}_s - (1-x)\dot{Q}_{rad} \tag{3}$$

$$T_c = xT_{c1} + (1-x)T_{c1} \tag{4}$$

where $\dot{\mathrm{E}} = \frac{\mathrm{V}^2}{\mathrm{R}}$ is the energy input (electrical); $\dot{\mathrm{Q}}_{\mathrm{conv}} = \mathrm{h_t A_{surf}(T_c - T_{amb})}$ is heat transfer by convection; $\dot{\mathrm{Q}}_{\mathrm{s}} = \mathrm{sk_s(T_c - T_s)}$ is heat transfer by conduction(the coil is considered as a disk on a semi-infinite medium which is the solder);

$\dot{\mathrm{Q}}_{\mathrm{rad}} = \sigma\mathrm{A_{surf}}\left(\mathrm{T_c}^4 - \mathrm{T_{amb}}^4\right)$ is heat transfer by radiation;

$\dot{\mathrm{m}}_{\mathrm{pg}} = \mathrm{h_m A_{surf}}(\mathrm{C_{vT_c}} - \mathrm{C_{vT_{amb}}})$ is mass transfer by convection; Heat and mass transfer coefficients ($\mathrm{h_{t,\ ,,}}$ $\mathrm{h_{m,}}$) are calculated according to Churchill and Bernstein correlations for cross flow over cylinders[28]; $x = \frac{L_{wet}}{L_{total}}$ & $1 - x$ are fractions of the wet and dry zone respectively where L_{wet} is dependent on the remaining mass on the heater coil.

Mass of PG

$$\frac{dm_{pg}}{dt} = -h_m A_{surf}\frac{M_{pg}}{Ru}\left(\frac{P_{vc_{pg\_mix}}}{T_c} - \frac{P_{vamb_{pg\_mix}}}{T_{amb}}\right) \tag{5}$$

Mass of Nicotine

$$\frac{\mathrm{dm_{nic}}}{\mathrm{dt}} = -\mathrm{h_{m\_nic}} \mathrm{A_{surf}} \frac{\mathrm{M_{nic}}}{\mathrm{Ru}} \left(\frac{\mathrm{P_{vc_{nic\_mix}}}}{\mathrm{T_c}} - \frac{\mathrm{P_{vamb_{nic\_mix}}}}{\mathrm{T_{amb}}}\right) \tag{6}$$

Based on the ideal solution assumption, the vapor pressure of both PG and nicotine in the mixture obeys Raoult's law as following:

Vapor Pressure

$$P_{v_{pg\_mix}} = Y_{pg} P_{v_{pg}} \tag{7}$$

$$P_{v_{nic\_mix}} = Y_{nic} P_{v_{nic}} \tag{8}$$

where the vapor pressure of PG $\mathrm{P_{v_{pg}}}$and that of nicotine $\mathrm{P_{v_{nic}}}$are calculated using Antoine equation. Moreover, while taking the main e-liquid component as PG, the model equally applies for more than just PG (PG and/or VG).

Temperature of the Solder

$$(mc_P)_s \frac{dT_s}{dt} = \dot{Q}_s - \dot{Q}_{cer} \tag{9}$$

where $\dot{Q}_{cer} = sk_{cer}(T_s - T_{cer})$ is heat transfer by conduction ceramic. The solder is considered as a disk on a semi-infinite medium, which is the ceramic.

Temperature of the Ceramic

$$(mc_P)_{cer} \frac{dT_{cer}}{dt} = \dot{Q}_{cer} - \dot{Q}_{tot} \tag{10}$$

where $\dot{Q}_{tot} = \frac{1}{Rt_{tot}}(T_{cer} - T_{amb})$ is the total heat loss from the ceramic to the surroundings. The heat loss is through conduction to the steel wool and to the housing, free convection from the housing to the surrounding, and radiation from the housing to the surrounding. Heat losses are represented as thermal resistances.

As mentioned in the above section, each part of the model requires inputs to get predicted outputs. The inputs of the evaporation part of the model are the following:

- Puff topography (puff duration, flow rate, inter-puff interval, puff number)
- Design Features:
    - Electrical power input
    - Nicotine Concentration
    - Air flow tube geometry
    - Heater element dimensions and mass
    - Mass and geometric properties of the components of the atomizer
- Thermodynamic and transport kinetic properties of air, and of E-liquid components (PG, VG, and nicotine)

Puff Topography and two of the design features (electrical power input, and nicotine concentration) can be varied by the user. The other design features were readily obtained by reverse engineering the different ECIG designs used.

Thermodynamic and transport kinetic properties were taken from literature and are given in Table 1. However, in the literature there is variation of some of these properties. A sensitivity analysis, which is done to study the effect of this variation on the predicted variables, is described in the following chapter.

The outputs of the evaporation model are:

- Temperature of the heating element
- Temperature of the Air
- Properties of the vapor
    - Temperature
    - Vapor pressure
    - Mass transfer coefficient
- Mass Evaporated

  - PG vapor
  - VG vapor
  - Nicotine Vapor

The temperature of the mass evaporated just at the vicinity of the heating element is the temperature of the heating element. The mass evaporated symbolizes the theoretical upper limit, or “potential mass” emitted from a given puffing session.

Air $M_{air} = 28.97 \times 10^{-3}$ $\rho_{air} = 0.995,\ c_p = 1.009 \times 10^3,\ \mu = 208.2 \times 10^{-7}, v = 20.92 \times 10^{-6}\ k = 30 \times 10^3$ [28] $V_{m_{air}} = \frac{M_{air}}{\rho_{air}}$
Propylene Glycol $M_{PG} = 76.09 \times 10^{-3}, T_b = 461.3\ ,\ \Delta Hvap\ = 914 \times 10^3$ [29], $s = 36 \times 10^{-3}$ [30] $\rho_{PG} = 1.036 \times 10^3,\ c_p = 2.5 \times 10^3$ [30] $\log_{10} P_s = A - \frac{B}{T_s+C}$ (A = 6.07936, B = 2692.187, C = -17.94) [31] $V_{m_{PG}} = \frac{M_{PG}}{\rho_{PG}}$ $D = \frac{0.001\times10^{-19/2}\times {T_s}^{1.75}\times \sqrt[2]{\left(\frac{M_{air}+M_{PG}}{M_{air}\times M_{PG}}\right)}}{P\times\left(\sqrt[3]{V_{m_{air}}}+\sqrt[3]{V_{m_{PG}}}\right)^2}$ [32]
Vegetable Glycerin $M_{VG} = 92.09 \times 10^{-3}, T_b = 563.15,\ \Delta Hvap\ = 974 \times 10^3$ [29], $s = 64 \times 10^{-3}$ [33] $\rho_{VG} = 1.261 \times 10^3,\ c_p = 2.37 \times 10^3$ [34] $\log_{10} P_s = A - \frac{B}{T_s+C}$ (A = 3.93737, B = 1411.531, C = -200.566) [35] $V_{m_{VG}} = \frac{M_{VG}}{\rho_{VG}}$ $D = \frac{0.001\times10^{-19/2}\times {T_s}^{1.75}\times \sqrt[2]{\left(\frac{M_{air}+M_{VG}}{M_{air}\times M_{VG}}\right)}}{P\times\left(\sqrt[3]{V_{m_{air}}}+\sqrt[3]{V_{m_{VG}}}\right)^2}$ [32]
Nicotine $M_{nic} = 162.2 \times 10^{-3}, T_b = 520.15,\ s = 38.61 \times 10^{-3}$ [36] $\rho_{nic} = 1.01 \times 10^3$[36] $\log_{10} P_s = A - \frac{B}{T_s+C}$ (A = 3.60721, B = 1433.766, C = -121.387) [37] $V_{m_{nic}} = \frac{M_{nic}}{\rho_{nic}}$ $D = \frac{0.001\times10^{-19/2}\times {T_s}^{1.75}\times \sqrt[2]{\left(\frac{M_{air}+M_{nic}}{M_{air}\times M_{nic}}\right)}}{P\times\left(\sqrt[3]{V_{m_{air}}}+\sqrt[3]{V_{m_{nic}}}\right)^2}$ [32]

Table 1. Thermo-physical properties of air, propylene glycol, vegetable glycerin, and nicotine.Values of M, the molecular weight in kg/mol; T_b , the normal boiling point in K; ΔH_{vap} , the specific latent heat of vaporization in J/kg; s, the surface tension in N/m; ρ, the density in kg/m^3; c_p , the specific heat capacity in J/kg.K; μ , the viscosity in N.s/m^2; v, the kinematic viscosity in m^2/s; k, the conductivity in W/m.K; V_m, the molar volume in m^3/mol; T_s , the temperature of the heating element in K; P_s , the vapor pressure in bar; D, the diffusivity in air in m^2/s .

C. Simplified Model

A simplified model of the evaporation model was developed in order to be able to perform dimensional analysis on the governing equations mentioned above. Dimensional analysis is vital for capturing the main parameters that mostly affect the predicted variables from the model: the temperature of the heater coil and the evaporation rate of e-liquid and nicotine. The main assumptions that are taken for simplification are as follows:

- The solder is lumped into the control volume of the heater coil
- The ceramic is taken to remain at room temperature

Based on the above assumptions, instead of having three energy equations to get temperature of coil, solder, and ceramic, there will be only one energy equation to get the temperature of the coil as following:

$$(\mathrm{mc_P})_{\mathrm{total}}\frac{\mathrm{dT_c}}{\mathrm{dt}} = \dot{\mathrm{E}}\text{-}(\mathrm{h_t A_{surf}} + 2\mathrm{sk_2})^*\left(\mathrm{T_c}\text{-}\mathrm{T_\infty}\right) + \mathrm{h_{fg}}^*\frac{\mathrm{dm_{PG}}}{\mathrm{dt}} \qquad (11)$$

The mass conservation equations of PG and nicotine stay the same as equations 5&6.

D. Governing Dimensionless groups

The simplified energy equation (Eq.11) and mass conservation equations of PG and nicotine (Eq. 5 &6) can be non-dimensionalized using the scheme shown in Table 2.

Variable	Dimensionless Form
Time	$t^* = \frac{t}{(T_b - T_\infty)(mc_P)_{total}/\dot{E}}$
Coil Temperature	$T_c^* = \frac{T_c - T_\infty}{T_b - T_\infty}$
Vapor Concentration	$C_T^* = \frac{C_T - C_{T_\infty}}{C_{Tb} - C_{T_\infty}}$
PG Evaporation Rate	$\left(\frac{dm_{pg}}{dt}\right)^* = \frac{\frac{dm_{pg}}{dt}}{h_{m\_pg}A_{surf}\,(C_{Tb\_pg} - C_{T_\infty\_pg})/Y_{pg}}$
Nicotine Evaporation Rate	$\left(\frac{dm_{nic}}{dt}\right)^* = \frac{\frac{dm_{nic}}{dt}}{h_{m\_nic}A_{surf}\,(C_{Tb\_nic} - C_{T_\infty\_nic})/Y_{nic}}$

Table 2.Variables in dimensionless form

Dimensionless Constants	Physical Meaning
$c_1 = \frac{(T_b - T_\infty)\left(h_t A_{surf} + 2sk_2\right)}{\dot{E}}$	Thermal energy flux relative to energy input flux
$c_2 = \frac{h_{fg} h_m A_{surf}(C_{T_b} - C_{T_\infty})}{\dot{E}}$	Latent energy flux relative to energy input flux
$c_3 = Y_{nic}$	Nicotine Mole Fraction

Table 3.Dimensionless constants

The resulting equations for the dimensionless temperature and evaporation rate of PG and nicotine are:

$$\frac{dT_c^*}{dt^*} = 1 - c_1 * T_c^* + c_2\left(\frac{dm_{pg}}{dt}\right)^* \tag{12}$$

$$\left(\frac{dm_{pg}}{dt}\right)^* = -(1 - c_3)C_T^* \tag{13}$$

$$\left(\frac{dm_{nic}}{dt}\right)^* = -c_3 C_{T\_nic}^* \tag{14}$$

where the dimensionless groups c_1–c_3 and their physical interpretations are given in Table 3.

In order to validate the dimensionless parameters and the assumptions taken for simplifying the model, values of temperature and mass flux of PG (per second) vs. time and temperature* and mass flux* vs. time* were predicted for four conditions from the original model (not simplified) and shown in Figure 6 and Figure 7 respectively. In the four conditions, the design features and the user behavior were changed in a way such that c1 through c3 remain the same for the four conditions. The parameters changed and the corresponding dimensionless constants in each of the four conditions are showed in Figure 4 and Figure 5. To get reliable dimensionless parameters, conditions of same c1 through c3 should give same temperature* and mass flux* vs. time*.

Condition	Description	Dimensionless Constants
1	Baseline Condition	c1=0.4; c2=1.2; c3=0.0081
2	Change conduction shape factor, mass of CV1, and ambient temperature	c1=0.4; c2=1.2; c3=0.0081
3	Change power input, flow, and conduction shape factor	c1=0.4; c2=1.2; c3=0.0081
4	Change power input, coil surface, and conduction shape factor	c1=0.4; c2=1.2; c3=0.0081

Figure 4.Parameters changed and the corresponding dimensionless constants in each of the four conditions.

Cond	$\dot{E}$	T_∞	$T_b - T_{amb}$	$C_b - C_{amb}$	h_t h_m	A_{surf}	sk_2	$(mc_P)_t$
1	1	1	1	1	1	1	1	1
2	1	1.07	0.87	0.99	1	1	1.26	1.14
3	1.44	1	1	1	1.44	1	1.44	1
4	2.27	1	1	1	1	2.27	2.27	1

Figure 5.Normalized values of the parameters changed in the four conditions relative to the baseline condition (Condition 1)

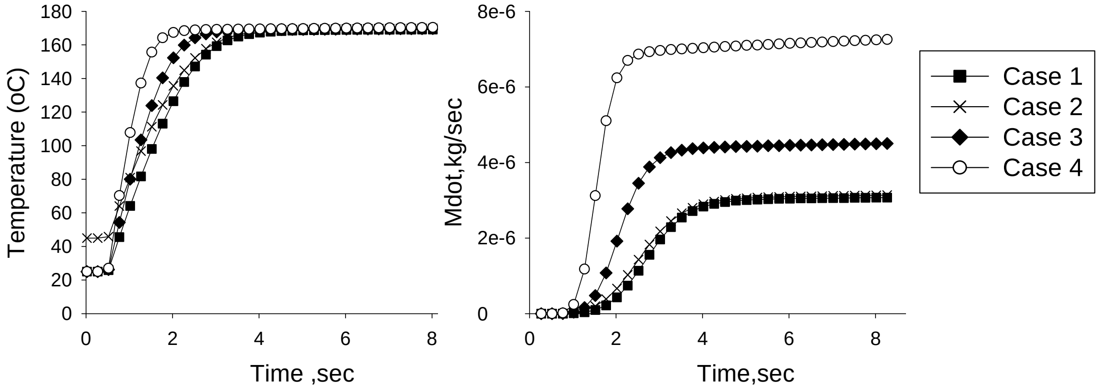

Figure 6.Temperature and evaporation rate vs. time for the four conditions

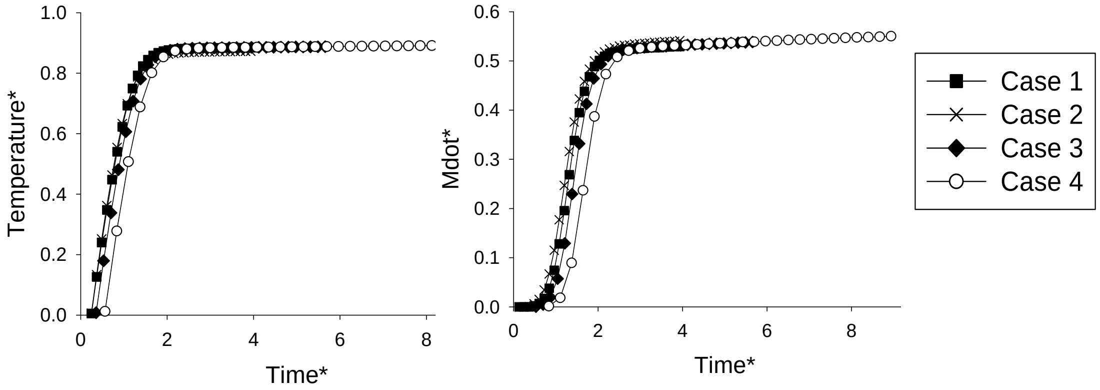

Figure 7.Temperature* and evaporation rate* vs. time* for the four conditions.

While the dimensionless constants are derived from the equation in the simplified model and the four conditions were predicted from the original model, varying some design features and user behavior keeping c1 through c3 constant gives different temperatures and mass flux but same temperature* and mass flux*(Figure 6 and Figure 7). This shows that the simplifying assumptions are valid and the dimensionless parameters are reliable.

Using the dimensionless analysis, it is effective to elucidate the main parameters affecting temperature and evaporation rate in three constants embodying the effect of puff flow, cartridge geometry, nicotine concentration and power input.

E. Mixing Model

The mixing model is the connecting model between the evaporation and condensation model. It is developed to get the temperature of air-vapor mixture, which will leave the heater coil and enter the mouthpiece. Control volume 4 is taken just after the heater coil where the vapor and the drawn air are mixed. Figure 8 shows what is happening at the boundary layer of control volume 4. The steady-flow energy equation is as follows:

Temperature of the mixture

$$\dot{Q}_{conv} + \dot{m}_a h_{a,i} + \dot{m}_v h_{v,i} - \dot{m}_a h_{a,o} - \dot{m}_v h_{v,o} = 0 \qquad (15)$$

Taking air and vapor as ideal gases with constant specific heats and knowing that $T_{a,i} = T_{amb}$; $T_{v,i} = T_c$, the above equation simplifies to :

$$\dot{Q}_{conv} = \dot{m}_a c_{P_a}\left(T_{mix} - T_{a,i}\right) + \dot{m}_v c_v (T_{mix} - T_{v,i}) \qquad (16)$$

$\dot{Q}_{conv}$ as mentioned above is the heat transfer by convection (from the coil to the air).

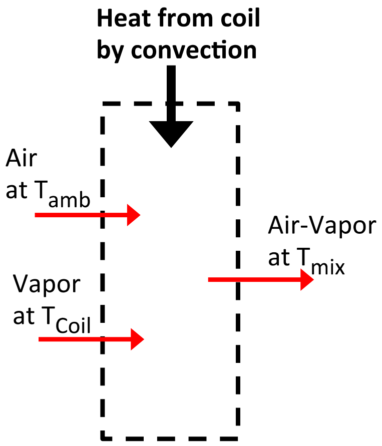

Figure 8.Schematic Diagram of Control Volume 4

The inputs of the mixing model are the outputs of the evaporation model. As for the outputs, they are as following:

- Temperature of the air-vapor mixture
    - Thermodynamic and transport kinetic properties of air at the above computed temperature.
- Mass of the air-vapor mixture (total and for each component)

CHAPTER III

MATERIALS AND METHODS

A. Numerical Solution

The resulted series of coupled differential equations are numerically solved in the Matlab® computing environment using a time-explicit algorithm, in increments of 0.01 ms. Results were checked for independence of time increment.

1. Sensitivity Analysis

There is variation in the reported values of several physical properties used in the calculations. Sensitivity of the key predicted variables – the coil temperature, evaporated PG and evaporated nicotine – was computed using a Monte Carlo approach. The variation is in the latent heat of evaporation of PG, vapor pressure of both PG and nicotine. The variation in the latent heat was from 850 to 934 KJ/mole [30, 31, 33]. Also, there were four equations found in the literature to compute PG vapor pressure, and five equations for nicotine. The equations are given in Appendix A.

Monte Carlo approach was used to generate 300 values of PG latent heat of vaporization. These values fall in the above range of latent heat and are of uniform distribution. With each of the 300 values of PG latent heat, different PG and nicotine vapor pressure equations were uniformly chosen from the equations found in the literature. The result of varying the above properties simultaneously on the key predicted variables- the coil temperature, evaporated PG and evaporated nicotine- is shown in Table 4.

Predicted Variable	Range	Min	Max	Mean	Std. Deviation	%Coefficient of Variance
Coil Temperature (K)	8.34	428.7	437.04	431.60	2.84	0.66
Evaporated PG (mg)	21.08	196.5	217.65	208.86	5.34	2.56
Evaporated nicotine (mg)	0.28	0.66	0.94	0.77	0.08	9.99

Table 4.Effect of varying several physical properties on key predicted variables.

For all the conditions, the predicted variables (coil temperature and mass evaporated of PG and that of nicotine) were sensitive to changing the above properties. However, the range of variation in the variables predicted was in the acceptable range (not more than 10 %).

B. Empirical Validation

To validate the model, a series of experiments were performed to compare measured total particulate matter (TPM) and nicotine yields to predicted evaporated total mass and nicotine.

1. Experimental Setup

The experimental setup for generating ECIG aerosol from one type of ECIG (prefilled cartomizer) is illustrated in Figure 9. A custom-designed digital laboratory-smoking machine at the American University of Beirut was used to generate ECIG aerosol for various ECIG design and puff topography conditions .For each experiment, the mouth end of the ECIG cartridge was connected by a 5 cm long Tygon® tube (ID) to a polycarbonate filter holder that contained a Gelman Type A/E 47 mm glass fiber filter. In preliminary experiments, we found that losses in the tubing connecting the ECIG cartridge to the filter pad were negligible.

The ECIG cartridge voltage was controlled using a regulated DC power supply, with 0.01V resolution.

TPM was determined gravimetrically by weighing the filter pad and holder before and after each sampling session. For nicotine measurements, filters were quantified and analyzed by GC-MS in accordance with the method presented by Siegmund et al. [38]with some adjustments that is illustrated in Saleh, R., & Shihadeh, A. [39]. The nicotine assay is not yet quantitative but is capable of providing relative yields

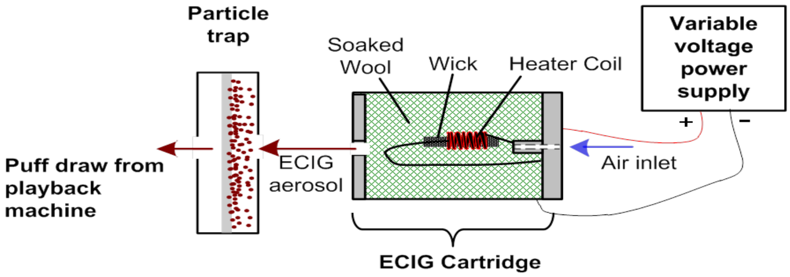

Figure 9.Experimental Setup

2. Experimental Matrix

The experiments needed to validate the model include varying the voltage of the power unit, changing the nicotine concentration in the E-liquid, and using three different ECIG designs. The key features of each ECIG design with its corresponding adjustments to the model are stated in Table 5. In addition to changing product features, the experiments also involve varying the puff topography including duration, inter-puff interval and flow which are all shown in Table 6. All experimental conditions are shown in Table 7.

ECIG	Description	Model Adjustments
Atomizer Dripper	E-liquid is dripped directly onto the horizontal heater coil, the coil is in the atomizer, a distinct piece from the mouthpiece (Resistance=2.7 ohms)	This design is the one used for the preliminary model
V4L Prefilled Cartridges (1&2)	One Vertical heater coil surrounded with poly-fill fiber holding the e-liquid, the coil is integrated within the mouthpiece. (Resistance=3.3 ohms for (1) and 3.7 ohms for (2))	Heat and mass transfer coefficients are calculated according to correlations for flow over isothermal plate (The coil is vertical instead of horizontal)
Smoktech Dual Coil	Two parallel horizontal heater coils surrounded with poly-fill fiber holding the e-liquid, the coil is integrated within the mouthpiece. (Total Resistance=3.2 ohms)	Two energy and two mass conservation equations, one for each heater coil (There are two coils instead of one; two surfaces to evaporate on instead of one)

Table 5.Operational Features of the ECIGs used with their corresponding model adjustments.

Cartridges	Analysis of factors affecting TPM & Nicotine Yields				
V4L Prefilled Cartridges (1&2)	Puff Duration	Flow Rate	Nicotine Concentration	Voltage & Resistance	Inter-puff Interval
Smoktech Dual Coil	Puff Duration	Flow Rate	Nicotine Concentration		
Atomizer Dripper	Design Features				

Table 6.Varied Parameters in the Experiments

Cond	ECIG Type	Voltage (V)	Number of Puffs	Puff Duration (sec)	Flow (L/min)	Nicotine Concentration (mg/mL)
1	V4L Prefilled Cartridges (1)	3.30	15.00	2.00	2.00	18.00
2	V4L Prefilled Cartridges (1)	3.30	15.00	8.00	2.00	18.00
3	V4L Prefilled Cartridges (1)	5.20	15.00	2.00	2.00	18.00
4	V4L Prefilled Cartridges (1)	3.30	15.00	4.00	1.00	18.00
5	V4L Prefilled Cartridges (1)	3.30	15.00	8.00	1.00	18.00
6	V4L Prefilled Cartridges (1)	3.30	15.00	4.00	2.00	18.00
7	V4L Prefilled Cartridges (1)	5.20	5.00	8.00	1.00	18.00
8	V4L Prefilled Cartridges (2)	3.30	15.00	2.00	2.00	18.00
9	V4L Prefilled Cartridges (2)	3.30	15.00	8.00	2.00	18.00
10	V4L Prefilled Cartridges (2)	5.20	15.00	2.00	2.00	18.00
11	V4L Prefilled Cartridges (2)	3.30	15.00	4.00	1.00	18.00
12	V4L Prefilled Cartridges (2)	3.30	15.00	8.00	1.00	18.00
13	V4L Prefilled Cartridges (2)	3.30	15.00	4.00	2.00	18.00
14	V4L Prefilled Cartridges (2)	5.20	5.00	8.00	1.00	18.00
15	V4L Prefilled Cartridges (2)	5.20	5.00	8.00	1.00	36.00
16	V4L Prefilled Cartridges (2)	3.30	15.00	4.00	1.00	36.00
17	V4L Prefilled Cartridges (2)	3.30	5.00	4.00	1.00	0.00
18	V4L Prefilled Cartridges (2)	3.30	10.00	4.00	1.00	0.00
19	V4L Prefilled Cartridges (2)	3.30	15.00	4.00	1.00	0.00
20	Smoktech Dual Coil	3.30	15.00	2.00	1.00	0.00
21	Smoktech Dual Coil	3.30	15.00	4.00	1.00	0.00
22	Smoktech Dual Coil	3.30	15.00	8.00	1.00	0.00

23	Smoktech Dual Coil	3.30	15.00	2.00	1.00	18.00
24	Smoktech Dual Coil	3.30	15.00	4.00	1.00	18.00
25	Smoktech Dual Coil	3.30	15.00	2.00	1.00	36.00
23	Smoktech Dual Coil	3.30	5.00	4.00	1.00	36.00
24	Smoktech Dual Coil	3.30	15.00	2.00	2.00	18.00
25	Smoktech Dual Coil	3.30	15.00	4.00	1.00	9.00
26	Atomizer Dripper	3.40	1.00	8.00	1.00	18.00
27	Atomizer Dripper	3.40	2.00	8.00	1.00	18.00

Table 7. Experimental Conditions

CHAPTER IV

RESULTS

A. Theoretical results

Figure 10 shows predicted temperature and nicotine flux within two 8-s puffs and their response to a change in flow and in voltage distinctly. Thus, effect of puff duration, flow and voltage could be studied. The flow and voltage in the three graphs is 1 l/min and 3.3 V unless otherwise noted.

1. Effect of puff duration

As shown in the lower graph Figure 10, the first quarter of the two-8 sec puffs represents the transient state of the system where its properties are constantly changing with time .The system here refers to the heating element and the liquid surrounding it. In the remaining portion, the system reaches the steady state where all properties become stable as time progresses i.e. temperature of the heater coil, e-liquid and nicotine vapor pressures, and in turn, the evaporated e-liquid and nicotine flux. Thus, for shorter puff duration, a larger portion of the puff will fall in the transient state resulting in lower average evaporated e-liquid and nicotine flux.

2. Effect of Flow Rate

As shown in the middle graph Figure 10, nicotine flux was not affected by changing the puff flow rate. This can be explained by the fact that nicotine flux is dependent on both nicotine saturation vapor pressure and mass transfer coefficient (Eq.

6). While at higher flow rates the air is better able to carry away vapors from the heater coil surface (i.e. higher mass transfer coefficient), it is also better able to carry away heat, resulting in a lower heater coil temperature. Lower heater temperature in turn, leads to lower nicotine vapor pressure. For the flow regimes present in an ECIG cartridge, the effects of flow rate on convective mass transfer coefficient and on nicotine vapor pressure almost exactly offset one another, resulting in a nicotine flux that is very nearly independent of flow rate.

3. Effect of Voltage

Higher voltage resulted in higher nicotine flux. This is due to the fact that electrical power input (E) is proportional to the square of the voltage. Thus, increasing the voltage leads to higher E resulting in higher heater coil temperature according to the principle of energy conservation (Eq.1). This can be seen in the upper graph of Figure 10. The increase in temperature results in an increase nicotine vapor pressure and subsequently nicotine flux as mentioned in the preceding section.

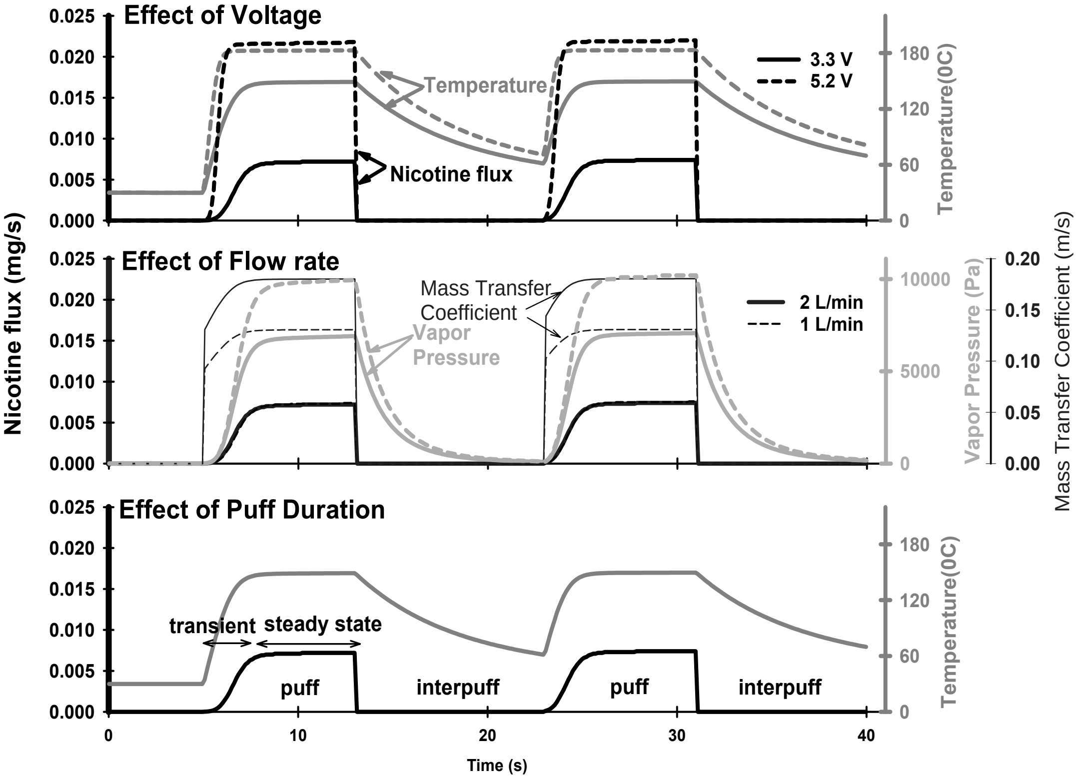

Figure 10.Predicted temperature and nicotine flux dynamics for two 8-s puffs with varying voltages and flow rates

4. Effect of Nicotine Concentration

Referring to Figure 11, higher nicotine concentrations in e-liquid resulted in higher evaporated nicotine flux but same evaporated e-liquid flux. This can be explained by the fact that even at higher concentrations (36 mg/mL), nicotine remains in trace amount relative to the overall mixture, and subsequently will have nearly no effect on the total mass evaporated.

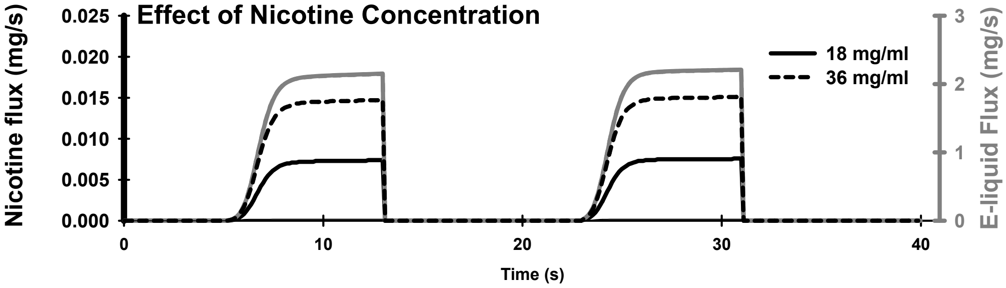

Figure 11.Predicted evaporated e-liquid and nicotine flux dynamics for two 8-s puffs with varying nicotine concentration

B. Experimental Results

The effect of nicotine concentration, flow rate, puff duration, and voltage on measured TPM and normalized nicotine yield per puff for two types of ECIG (V4L cartridges (1) & Dual Coils) is shown in Figure 12.The measured nicotine yields per puff were normalized by the condition that gave the highest value of nicotine per puff. The experimental measurements show the following:

- Higher nicotine concentration resulted in higher normalized nicotine yield per puff but same TPM per puff.
- Puff flow rate had no effect on neither TPM nor normalized nicotine yield.
- Greater puff duration resulted in disproportionately greater TPM and normalized nicotine yield per puff for both ECIGs.
- Higher voltages resulted in higher TPM and normalized nicotine yield per puff.
- For the same conditions, TPM and nicotine yield of dual coil is higher than that of V4L prefilled cartridges.

- TPM and normalized nicotine yield responded similarly upon varying the above parameters except the nicotine concentration.

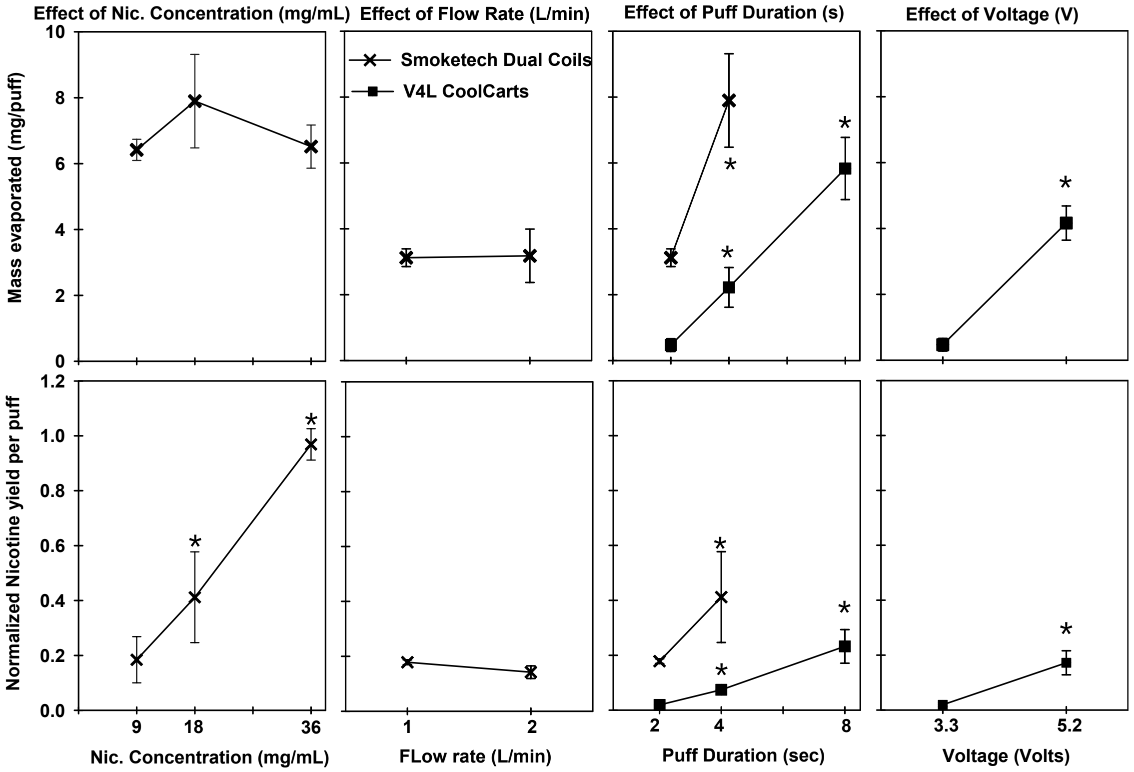

Figure 12.Measured TPM and normalized nicotine yield per puff (the baseline conditions for all data points presented are the following: puff duration: 2 seconds, flow rate: 1 l/min, voltage: 3.3 Volts apart for the effect of nicotine concentration results which were measured for a puff duration of 4 seconds; mean 95% CI; * indicated $p<0.05$ relative to baseline)

C. Model validation

From the above two sections, the experimental results concerning the effect of puff duration, flow rate, voltage, and nicotine concentration were well predicted and explained theoretically by the mathematical model. Moreover, predicted total mass and nicotine evaporated for all the experimental conditions mentioned in Table 7 were obtained, normalized by the condition that gave the maximum predictions of total mass and nicotine evaporated, and compared to the normalized measured data of TPM and nicotine yield under the same conditions. As seen in Figure 13, the values show that the normalized predicted and measured results exhibit an overall linear trend with high coefficients of determination of R^2 =0.97 & 0.96 with slopes of 0.96 and 0.99 for total mass and nicotine respectively. Hence, the different factors affecting nicotine emissions are well captured in the mathematical model.

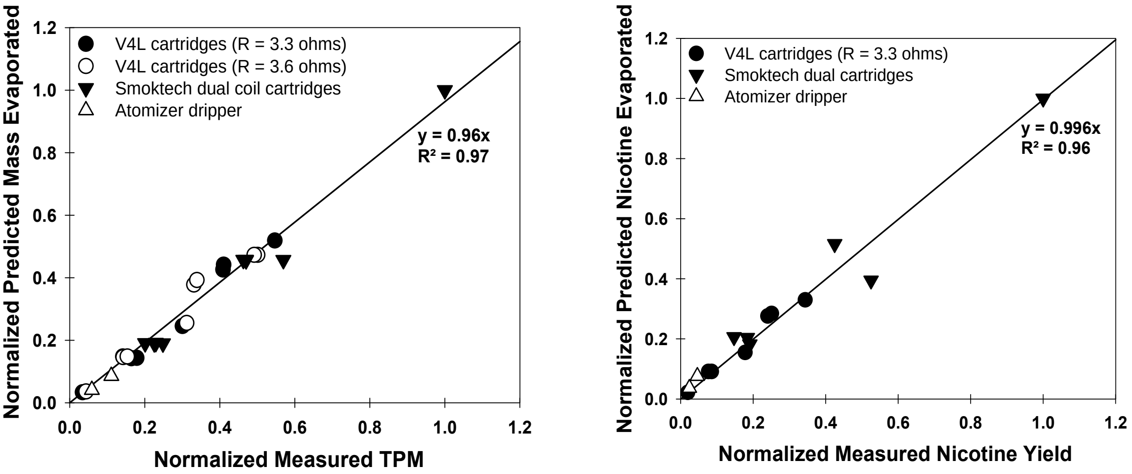

Figure 13.Normalized Predicted total mass and nicotine evaporated vs. normalized measured (TPM) and nicotine yield respectively for all the experimental conditions stated in Table 7

Figure 14 shows that the quantitative predicted total mass evaporated and measured TPM for the above conditions exhibit an overall linear trend with high coefficient of determination of R^2=0.97 with slope of 2.2. This signifies that the model predicts an average value of evaporated mass that is roughly double the value of inhaled TPM. This is expected because, as mentioned above, a fraction of the vapors is likely to condense on the internal surfaces of the mouthpiece; moreover in this work, the modeling effort focuses on the evaporation process and does not account for the condensation phenomena.

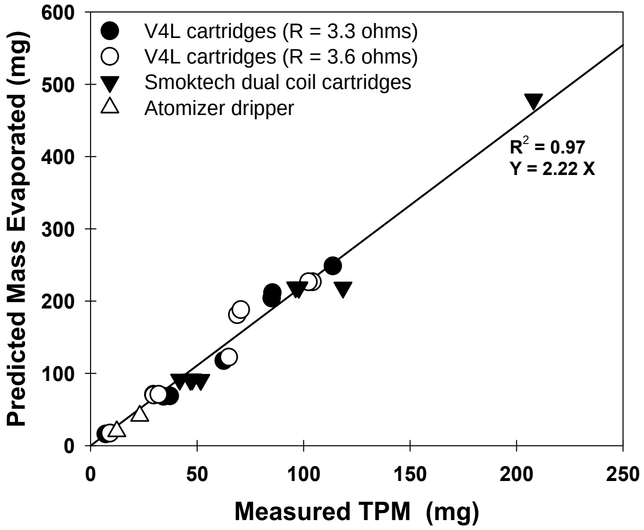

Figure 14.Predicted total mass evaporated vs. measured TPM for the experimental conditions stated in Table 7.

For conditions 1 through 7 that are mentioned in Table 7, normalized measured nicotine yield was highly correlated to normalized measured TPM (Figure 15; y=0.96x & R^2=0.98). These conditions include varying puff duration, flow rate, and voltage for the 7 conditions. This suggests that to a good first approximation, for a given e-liquid nicotine concentration, the nicotine yield can be taken as proportional to the amount of e-liquid vaporized.

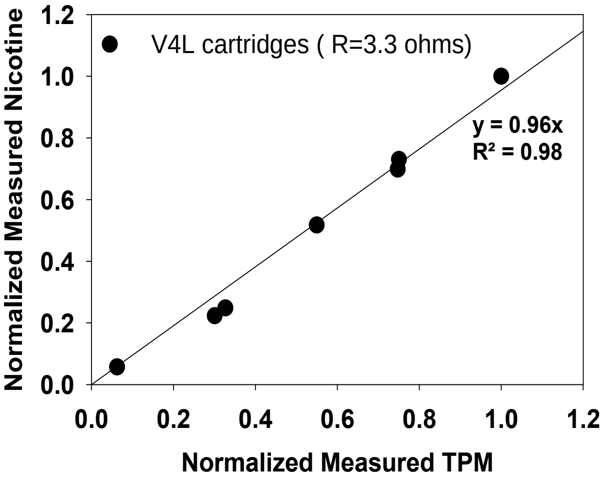

Figure 15.Normalized Measured Nicotine vs. TPM for the experimental conditions using V4L cartridges of R=3.3 ohms.

CHAPTER V

CONCLUSION

The mathematical model proved capable of predicting nicotine and TPM emissions from several ECIG designs that were utilized under a wide range of operating conditions. It also provided insight into the physical phenomena underlying the ECIG vaporization process. The mathematical model can be used to identify products that are likely to pose public health challenges (e.g., nicotine yield that is too low or too high) and then to guide selection of use conditions and product designs for subsequent human lab investigations.

Accounting for the ECIG condensation process can further refine the model in order to get an insight of the whole physical phenomena occurring in the ECIG. Thus, in addition to the mass evaporated from ECIG, the model will also be able to predict the TPM inhaled by the user after this refinement. Moreover, further work on nicotine analysis should be done to get quantitative nicotine yields instead of relative ones.

APPENDIX A

The equations found in literature to compute PG vapor pressure are as following:

- Clausius-Clapeyron Equation

$$ln\frac{P_S{}^*}{P_1} = \frac{\overline{\Delta H}_{vap}}{R} \times (\frac{1}{T_1} - \frac{1}{T_S}) \quad (\overline{\Delta H}_{vap} = 62 \times 10^3; P_1 = 34.47\ \ at\ T_1 = 310)\ [40]$$

$$ln\frac{P_c{}^*}{P_2} = \frac{\overline{\Delta H}_{vap}}{R} \times (\frac{1}{T_2} - \frac{1}{T_c}) \quad (\overline{\Delta H}_{vap} = 62 \times 10^3; P_2 = 86804.9\ \ at\ T_2 = 455)\ [40]$$

Antoine Equation

$$log_{10} P_s = A - \frac{B}{T_S + C}\ \text{(A=6.07936, B=2692.187, C=-17.94)}\ \ [31]$$

Derived Equation

$$\log_{10} \mathrm{P_s} = 9.33 - \frac{2970.9}{\mathrm{T_s}} + \log_{10}(133.3)\ (\mathrm{T}: 333 - 466\ \mathrm{K})\ \ [41]$$

The equations found in literature to compute nicotine vapor pressure are as following:

- Clausius-Clapeyron Equation

$$ln\frac{P_c{}^*}{P_1} = \frac{\overline{\Delta H}_{vap}}{R} \times (\frac{1}{T_1} - \frac{1}{T_c})\ (\overline{\Delta H}_{vap}{}^{**} = 55.299 \times 10^3; P_1 = 3786\ \ at\ T_1 = 406.9)[42]$$

$$ln\frac{P_c{}^*}{P_2} = \frac{\overline{\Delta H}_{vap}}{R} \times (\frac{1}{T_2} - \frac{1}{T_c})\ (\overline{\Delta H}_{vap}{}^{**} = 55.299 \times 10^3; P_2 = 33063\ at\ T_2 = 472.05)[42]$$

Antoine Equation

$$log_{10} P_c = A - \frac{B}{T_c + C}\ \ \text{(A=3.60721, B=1433.766, C=-121.387)}\ [37]$$

Derived Equations

$$P_c = \frac{101325}{760} \times 10^{172.8 - \frac{9492}{T_S} + 60.6\, log_{10}(T_S) + 0.0248 T_S}\ (T: 288 - 523K)\ [42]$$

$$P_c = \frac{101325}{760} \times 10^{8.0935 - \frac{2695.5}{T_c}}\ \ [40]$$

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