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Methodology for experimental research of heat and mass transfer processes during inhalation of e-cigarettes aerosols

Introduction

Electronic cigarettes (e-cigarettes, ECs) which are new technical devices for nicotine delivery through the respiratory system, are still poorly characterized regarding the aerosol properties and dynamics after leaving the EC and entering the respiratory tract. Lack of knowledge in this field constitutes a barrier that limits the ability to predict the lung deposition of EC-aerosol droplets and further analysis of safety and dangers related to EC mists inhalation.

The real-time characteristics of main EC-aerosol properties (e.g. size distribution of particulate phase) in different inhalation maneuvers and environmental conditions is necessary to better understand and describe the heat and mass transport processes. This should allow a better quantitative assessment of EC-aerosols penetration and deposition in different areas of the respiratory system (upper airways, tracheobronchial tree, alveoli) using computational methods.

This work is focused on the development and validation of the method of experimental testing of EC-aerosols to determine the impact of heat and mass transfer processes on their properties both during aerosol generation and penetration through the human respiratory tract.

The basic characteristics of EC-aerosol

ECs produce a highly concentrated mist of submicrometer liquid droplets suspended in the mixture of air and the vapor produced by heating of e-liquids. Formation of these droplets occurs on nanoparticles that serve as the centers of vapor condensation when the critical vapor supersaturation is achieved. According to the ECs` principles of operation, physical properties of aerosol released from ECs depend on several factors. The most important are the conditions in which the aerosol is formulated. The key role plays simultaneously the factors responsible for the intensity of e-liquid evaporation (i.e. construction and wattage of the heating element) but also for the dilution of vapor with the auxiliary air (i.e. dynamics of lung ventilation during aerosol inhalation, called the vaping topography) [*Odziomek et al., 2017; Sosnowski and Odziomek, 2018*].

EC-aerosol in the respiratory tract undergoes the further rapid changes in particle diameter due to evaporation or growth as it seeks equilibrium at the changing conditions of temperature and humidity. Droplets remaining for some period in the oral cavity can evaporate, the surrounding vapor may condense on droplets' surface and droplets may coagulate. Simultaneously, the vapor may be absorbed by the walls of the oral cavity which reduces the vapor partial pressure changing the driving force for evaporation/condensation processes [*Sosnowski and Odziomek, 2018*].

It is clear, that the properties and concentration of inhaled aerosol are dynamically altered during a relatively short period of aerosol residence in the upper airways, and this effect should have also a strong impact on droplets distribution and deposition after aerosol transfer to the lower airways. The unanswered question is how the vaping topography and manner of aerosol inhalation (e.g. mouth-hold period) influences the properties of droplets inside the respiratory tract. The puff volume from ECs may change between 30 and more than 350 cm^3. Also, the flow rate during puffing and the puffing time is significantly scattered among EC users (25÷100 cm^3/s and 0.7÷6.9 s, respectively) [*Robinson et al., 2015*].

For conventional cigarette smoke particles (CSPs), a number of *in vivo, in vitro* and numerical studies have been performed regarding the influence of heat and mass transfer processes during inhalation on CSPs properties. In summary, the hygroscopic growth of CSPs is around 1.5 at physiological temperature (37°C) and 99.5% of saturation humidity. [*Tang et al., 2012*] The hygroscopic growth of EC-aerosol droplets should be even stronger. The main components of e-liquids and aerosol droplets are propylene glycol (PG) and glycerin (VG), substances which have an affinity for water (humectants). Within the humid environment of the human respiratory tract the PG and VG should promote the hygroscopic growth of droplets, change in aerosol size distribution and - as a consequence - alteration of the regional particles deposition in the lungs. However, the accurate data concerning e-cigarettes dynamics in such conditions are very scarce due to measuring difficulties.

Measurement techniques and their applicability to EC-mist

The scarcity of information on particle size for ECs is due not only to their novelty, but also as a result of technical obstacles related to the measurement of highly-concentrated aerosols containing volatile particulate material.

The majority of published data have been obtained with instruments which require a high degree of aerosol dilution down to the operational range of aerosol concentration (e.g., differential mobility analyzer - DMA). This significantly affects the recorded results of size distribution and reduces the role of some dynamic processes (e.g. droplet coagulation). Another problem is that a high dilution required to perform such measurements may also cause a significant droplet evaporation. Accordingly, laser diffraction spectrometers seem to be more suitable for studies of concentrated EC-aerosols. The main advantage of this technique is that it requires no aerosol dilution, so the measurements can be done *in situ* and on-line, without any interference of the aerosol cloud. [*Sosnowski and Odziomek, 2018; Sosnowski and Kramek-Romanowska, 2015*]

Aerosol generation method in EC studies is often adapted from the methodology developed earlier for conventional cigarettes. [*Zhang et al., 2013*] Common systems in investigations of cigarettes and e-cigarettes use the "smoking machines" to generate (draw) and dilute the mainstream smoke/vapor samples to the experimental chamber. However, the characteristic inhalation maneuver in using e-cigarettes is different than in classic cigarettes, so smoking machines are not suitable for EC studies. It is associated with a different vaping topography and different value of internal aerodynamic resistance of cigarettes and their electronic counterpart [*Sosnowski and Kramek-Romanowska, 2015*]. Breathing simulators are more suitable for EC-aerosol testing since they have a better flexibility in programming of breathing dynamics.

Research methodology suitable for EC-aerosol testing must also take into account the specific properties of aerosols released from this source. The proposed methodology meets the relevant requirements and allows to measure changes of EC-aerosol properties in the following conditions:

- during interaction with the humid air with adjusted flow rate, which allows to change the time of interactions, the temperature and the humidity of the auxiliary air,
- under the simulated conditions of the human respiratory tract with variable aerosol residence time in the physiologically humid environment associated with inhalation pattern.

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Methodology

Aerosol source

Two models of electronic cigarette were tested: White (*Volish*) and iKonn (*Eleaf*). Both devices were filled the same e-liquid (PG/VG 1/1 v/v). Heating of e-liquid in both ECs was activated by manually pressing the button located on their bodies.

Particle size measurement technique and aerosol drawing system

Particle size distribution of aerosol droplets emitted from ECs was determined with *Spraytec* laser diffractometer (*Malvern Instruments*, UK) with the measuring range of 0.1 - 900 µm and 100 Hz sampling rate. The measuring system was equipped with the commercial 'inhalation chamber' accessory, where EC was connected to the system via the standard *US Pharmacopeia* (USP) inlet required for the correct horizontal orientation of ECs. The air flow through ECs was produced by either (1) the vacuum pump (*Vacuubrand*, Germany) – for the constant flow of 10 dm^3/min, or (2) the breathing simulator (*ASL 5000XL, Ingmar Medical*, USA) – for the programed inhalation pattern. Breathing profiles generated in the ASL device reflected two most representative puff topographies, Table 1 [*Robinson et al., 2015*]. The *Auxiliary Gas Exchange Cylinder* (AGEC) was used to protect the ASL against contamination with aerosol.

Tab. 1. EC Puffing topography

Puff symbol	Puff duration [s]	Flow rate [ml/s]	Puff volume [ml]	Puff interval [s]	Puff period [s]
A	3.7	39	144	48.7	52.4
B	6.9	44	304	47.7	54.6

EC-aerosol conditioning

In the first case (1), EC-aerosol was introduced into the air conditioned by medical air humidifier *MR 730* (*Fisher & Paykel Healthcare*, UK), commonly used for the moisturizing the air delivered to artificially ventilated patients. The device consists of the heated chamber filled with water and the pipe with the heating wire. Air temperature can be controlled and adjusted both in the heated chamber but also on the entire length of the pipe connecting the heated chamber of the humidifier and the *Spraytec* inhalation chamber (Fig. 1).

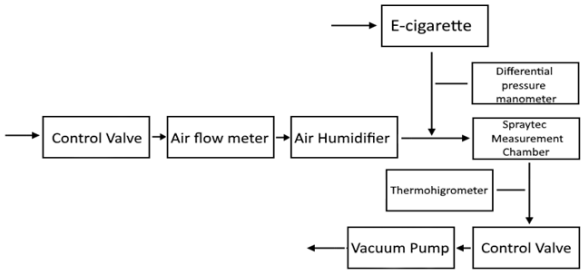

Fig. 1. Scheme of the experimental setup (1)

The proper adjustment of the temperatures and the air flow rate through this system (with two regulating valves) allows to control the air humidity of the residence time. In consequence, the time of interaction between the humidified air and EC-aerosol can be also adjusted (approximately to 0.5 s). EC is connected to the system between the humidifier chamber and the inhalation (i.e. measuring) chamber of Spraytec device. The aerosol is drawn from the EC due to the negative pressure generated by the pump. Measurement of the pressure drop directly before the EC mouthpiece allows to calculate the flow rate of the external air through the EC as the specific aerodynamic resistance of the EC is known. The flow rate of external air through the EC can be adjusted by the control valves.

In the experiments with breathing simulator (2), the aerosol released from ECs is first introduced into the heated chamber filled with water (37°C, saturation conditions) and then exhaled into the *Spraytec* measurement chamber (Fig. 2). Check valves allows to first draw out aerosol from the EC during inhalation and then removing it from the conditioning chamber to the *Spraytec* measurement chamber during exhalation.

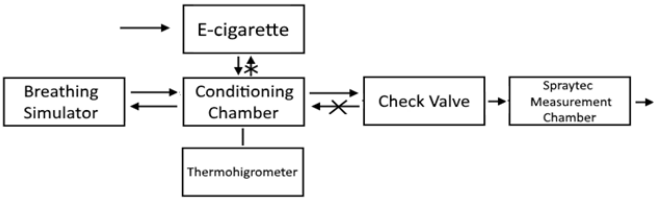

Fig. 2. Scheme of the experimental setup (2)

Example results

First results obtained in the developed measuring systems indicate significant differences in the volume median diameter (VMD) of droplets in EC-aerosols mixed with the air with 30 and 85% RH (at 37°C). A strong effect is observed when the relatively small stream of air (0.75 dm^3/min) is drawn through the EC (VMD = 0,72±0,02 µm and 1,13±0,07 µm respectively).

Application of the described methodology allows to detect differences in VMD of aerosols generated at different puffing topographies as well. For the most typical case (A in Table 1) VMD of the aerosol exhaled from the conditioning chamber is close to 2.5 µm whereas in the second case B (longer and deeper puffs) VMD is equal almost 3.5 µm. Both results suggest a significant increase in median droplet size in comparison to the aerosol released directly from EC (VMD = 0.6 µm).

Conclusions

The initial results indicate the usefulness and applicability of developed methodology for EC-aerosol testing for a deeper understanding of the influence of the simultaneous heat and mass transfer processes during EC-aerosol formation, inhalation and movement in the human respiratory tract.

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