Regulatory Toxicology and Pharmacology xxx (2017) 1–10

Contents lists available at ScienceDirect

Regulatory Toxicology and Pharmacology

journal homepage: www.elsevier.com/locate/yrtph

Assessment of tobacco heating product THP1.0. Part 2: Product design, operation and thermophysical characterisation

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ARTICLE INFO

Article history:
Received 17 April 2017
Received in revised form
14 August 2017
Accepted 10 September 2017
Available online xxx

Keywords:
Tobacco heating product
Combustion
Next generation products
THP1.0
Thermophysical assessment
Preclinical assessment

ABSTRACT

A novel tobacco heating product, THP1.0, that heats tobacco below 245 °C is described. It was designed to eliminate tobacco combustion, while heating tobacco to release nicotine, tobacco volatiles and glycerol to form its aerosol. The stewardship assessment approach behind the THP 1.0 design was based on established toxicological principles. Thermophysical studies were conducted to examine the extent of tobacco thermal conversion during operation. Thermogravimetric analysis of the tobacco material revealed the major thermal behaviour in air and nitrogen up to 900 °C. This, combined with the heating temperature profiling of the heater and tobacco rod, verified that the tobacco was not subject to combustion. The levels of tobacco combustion markers (CO, CO_2, NO and NO_x) in the aerosol of THP1.0 were significantly lower than the levels if there were any significant pyrolysis or combustion. Quantification of other tobacco thermal decomposition and evaporative transfer markers showed that these levels were, on average, reduced by more than 90% in THP1.0 aerosol as compared with cigarette smoke. The physical integrity of the tobacco consumable rod showed no ashing. Taken together, these data establish that the aerosol generated by THP1.0 is produced mainly by evaporation and distillation, and not by combustion or pyrolysis.

1. Introduction

Cigarette smoking is one of the leading preventable causes of human diseases such as lung cancer, chronic obstructive pulmonary disease and cardiovascular disorders (US DHHS, 2014). Most smoking-related diseases are not caused by nicotine but by toxicants present in the inhaled smoke (Farsalinos and Le Houezec, 2015), many of which form during the combustion and pyrolysis of the tobacco (Baker, 2006).

When a cigarette is lit, the tobacco burns to form smoke containing more than 6500 compounds (Rodgman and Perfetti, 2013), approximately 150 of which are thought to be toxicants (Fowles and Dybing, 2003). While modifying the way in which a cigarette burns has proved to be technically limited in its effects to significantly reduce the health risks based on current scientific understanding and available technologies (Baker, 2006; McAdam et al., 2012), tobacco-heating products (THPs), where a sample of tobacco is heated to temperatures sufficient to vaporize volatile compounds including nicotine into an inhalable aerosol, but not high enough to burn the tobacco, have the potential to significantly reduce the levels of combustion-derived toxicants in the generated aerosol (Schorp et al., 2012; Zenzen et al., 2012; Forster et al., 2015; Smith et al., 2016). Furthermore, heating tobacco at temperatures below those found in tobacco burning cigarettes have been shown to reduce the mutagenicity of the smoke condensate (White et al., 2001).

Several ways to deliver aerosol by heating tobacco have been described in both patents and the literature. Studies of first-generation electrically heated cigarettes (EHCs) indicated that approximately two-thirds of aerosol constituents were reduced by at least 50% and many were reduced by more than 90%, as compared with conventional cigarette smoke; however, formaldehyde yields increased (Stabbert et al., 2003). Second-generation EHCs included ammonium magnesium phosphate (AMP) in the cigarette paper to reduce the formation of formaldehyde (Moennikes et al., 2008). Typical smoke exposure-related changes in rat lung were less pronounced after exposure to aerosol from a second-generation EHC with AMP than to aerosol from the first-

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https://doi.org/10.1016/j.yrtph.2017.09.009

generation EHC or smoke from the conventional reference cigarette, when compared on a particulate matter or nicotine basis (Moennikes et al., 2008).

More recent characterizations of an electrically heated cigarette smoking system (originally EHCSS, now an updated version) found that the aerosol generated by the products was distinctly different from the smoke of a conventional cigarette (Zenzen et al., 2012; Schorp et al., 2012; Smith et al., 2016). With very few exceptions, these electrically heated tobacco products demonstrated a substantial reduction in the toxicological activity of the aerosol versus a conventional cigarette when smoked with comparable puffing intensities or at comparable nicotine yields. Based on an overall weight-of-evidence approach, the authors concluded that the product design could reasonably be expected to reduce the hazard relative to conventional cigarettes, and that smoking using the EHCSS or THS 2.2 would result in substantially reduced exposure to harmful and potentially harmful constituents (HPHCs) (Smith et al., 2016).

Such studies have led to commercially available THPs in some countries, including Eclipse/Revo, Ploom and iQOS. Each of these THPs uses a different heating method characterised by their heater configuration in relation to the tobacco bed or rod (inside vs external to the tobacco bed), the heating profile of the heater (temperature ramp rate, maximum temperature and duration of heating), and last but not least the way in which the tobacco material is specifically processed to work with low to moderate heating temperatures. Thus, it is necessary to understand how tobacco behaves under these different heating methods.

Broadly speaking, tobacco materials undergo four main thermal decomposition processes — dehydration, volatile release, pyrolysis and combustion — as determined by extensive pyrolysis studies conducted to understand the formation of smoke constituents in a burning cigarette in the 1970s and 1980s (summarized in (Baker, 1987)). Temperature changes during puffing were characterised by thermocouples and infrared probes inserted into the end of burning cigarette, and evolved gas concentrations were measured by mass spectrometry. This series of research established that the burning zone of the cigarette, which is oxygen-deficient and hydrogen-rich, comprises two regions: an exothermic combustion zone, and an endothermic pyrolysis/distillation zone. As air is drawn into the cigarette during a puff, O_2 is consumed by the combustion of carbonised tobacco, forming the products CO, CO_2 and H_2O alongside the release of heat that sustains the whole burning process. The temperatures in this combustion region reach as high as 950 °C, and are generated at rates of up to 500 °C/s. Immediately behind is the pyrolysis zone, where the temperatures are lower (200–600 °C) and the O_2 levels are low. Most of the smoke constituents are formed by endothermic processes in this region, and the resulting highly concentrated aerosol is drawn down the cigarette rod to form mainstream smoke during a puff (Baker, 1987).

More recently, pyrolysis experiments under simulated conditions of cigarette burning have been used to investigate mechanistic and kinetic aspects of tobacco combustion (Czégény et al., 2009; Várhegyi et al., 2010), as well as factors that affect the generation of known toxicants/volatiles including temperature, pyrolysis atmosphere and pH (Torikai et al., 2004). Studies have also modelled a burning cigarette using computational fuild dynamic algorithms (Rostami et al., 2003).

Tobacco is a nitrogen-rich plant material: its main components are hemicellulose, cellulose and lignin, while nitrogenous compounds comprise its major characteristic fractions. Thermogravimetric analysis (TGA) coupled with hyphenated detection tools, such as Fourier transform infrared (FTIR) spectroscopy for evolved gases and volatiles has been widely used to examine the thermal decomposition of the three key biomass components during the pyrolysis of different biomasses (Yang et al., 2006, 2007; Liu et al., 2008, 2013; Lee and Fasina, 2009). The results show that most of the plant material undergoes the following series of thermophysical and thermochemical processes when heated: moisture evolution, hemicellulose decomposition, cellulose decomposition, lignin degradation, and lastly charring. A low-temperature maximum is generally recorded on the derivative of the weight loss curve, indicating the first onset of thermal decomposition, which is usually above 200 °C and below 350 °C.

Several studies have specifically examined the thermal decomposition of tobacco by TGA (Wójtowicz et al., 2003; Oja et al., 2006; Barontini et al., 2013a, 2013b). In particular, Barontini et al. (2013a,2013b) developed multivariate deconvolution methodology to obtain quantitative data on key components of interest in gases evolved during TGA-FTIR analysis of tobacco at low heating rates. Analysis of the differential (rate of weight loss) thermogravimetric curves delineated four regions of weight loss: region I (30–120 °C), related to moisture release; regions II (120–250 °C) and III (250–370 °C), related to a two-stage thermal decomposition and evaporation phenomenon; and region IV (370–550 °C), related to a further thermal decomposition (in nitrogen) or to combustion (in air) of the residue obtained from the primary decomposition process Barontini et al. (2013a,2013b). They also obtained emission profiles of seven analytes (CO_2, CO, acetaldehyde, nicotine, phenol, isoprene, water, and glycerol) over the temperature range Barontini et al. (2013b).

Similarly, Liu et al. (2013) determined the composition of evolved volatiles from fast pyrolysis of tobacco stem by pyrolysis coupled with gas chromatography/mass spectrometry (Py-GC/MS) analysis, and investigated the evolution patterns of major products by TGA-FTIR and TGA-MS techniques. Furfural and phenol, generated from the depolymerization of cellulose, were the major products from low-temperature pyrolysis (~400 °C), whereas indene and naphthalene were the major products from high-temperature (~800 °C) pyrolysis. CO, CO_2, phenols, aldehydes, and ketones were released between 167 °C and 500 °C, whereas CO and CO_2 were the main gaseous products at temperatures >500 °C.

Recently, Cozzani et al. (2016) reported the use of two indicators for the detection of tobacco combustion: first, the presence of relevant quantities of NO_x in the aerosol that could not be formed from the decomposition of nitrates present in the original biomass/tobacco; and second, simultaneous evidence of a self-sustaining exothermic process. The latter indicator has been tested by Yan and Fujita (2016), who modelled the way in which tobacco is heated in a solid porous medium with an electrical heater embedded in the axial centre. The outcome of the modelling was a mathematical expression of the self-sustaining exothermic process, defined as $d^2T/dt^2 > 0$ and $dT/dt > 0$ in the range $T > 400$ K for the heated tobacco.

Regarding the design of THPs, it is important to characterise the heating processes within and to establish that little or no combustion takes place. To this end, Forster et al. (2015) used a bench-top tube furnace that heats tobacco between 100 and 200 °C to investigate low-temperature release for selected HPHCs typically associated with tobacco smoke. Among several targeted chemical compounds, seven toxicants (nicotine, CO, acetaldehyde, crotonaldehyde, formaldehyde, NNN and NNK) were quantifiable in the aerosol generated under the ISO machine-smoking protocol, but not at all temperatures examined. In the total aerosol phase collected, water was the largest measured component and seemed to be released mainly by evaporation, whereas between 100 °C and 200 °C, nicotine and some cigarette smoke compounds were released due to evaporative transfer or initial thermal decomposition from the tobacco blend.