World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:10, No:04, 2016

Modeling Aerosol Formation in an Electrically Heated Tobacco Product

Authors : Markus Nordlund, Arkadiusz K. Kuczaj

Abstract : Philip Morris International (PMI) is developing a range of novel tobacco products with the potential to reduce individual risk and population harm in comparison to smoking cigarettes. One of these products is the Tobacco Heating System 2.2 (THS 2.2), (named as the Electrically Heated Tobacco System (EHTS) in this paper), already commercialized in a number of countries (e.g., Japan, Italy, Switzerland, Russia, Portugal and Romania). During use, the patented EHTS heats a specifically designed tobacco product (Electrically Heated Tobacco Product (EHTP)) when inserted into a Holder (heating device). The EHTP contains tobacco material in the form of a porous plug that undergoes a controlled heating process to release chemical compounds into vapors, from which an aerosol is formed during cooling. The aim of this work was to investigate the aerosol formation characteristics for realistic operating conditions of the EHTS as well as for relevant gas mixture compositions measured in the EHTP aerosol consisting mostly of water, glycerol and nicotine, but also other compounds at much lower concentrations. The nucleation process taking place in the EHTP during use when operated in the Holder has therefore been modeled numerically using an extended Classical Nucleation Theory (CNT) for multicomponent gas mixtures. Results from the performed simulations demonstrate that aerosol droplets are formed only in the presence of an aerosol former being mainly glycerol. Minor compounds in the gas mixture were not able to reach a supersaturated state alone and therefore could not generate aerosol droplets from the multicomponent gas mixture at the operating conditions simulated. For the analytically characterized aerosol composition and estimated operating conditions of the EHTS and EHTP, glycerol was shown to be the main aerosol former triggering the nucleation process in the EHTP. This implies that according to the CNT, an aerosol former, such as glycerol needs to be present in the gas mixture for an aerosol to form under the tested operating conditions. To assess if these conclusions are sensitive to the initial amount of the minor compounds and to include and represent the total mass of the aerosol collected during the analytical aerosol characterization, simulations were carried out with initial masses of the minor compounds increased by as much as a factor of 500. Despite this extreme condition, no aerosol droplets were generated when glycerol, nicotine and water were treated as inert species and therefore not actively contributing to the nucleation process. This implies that according to the CNT, an aerosol cannot be generated without the help of an aerosol former, from the multicomponent gas mixtures at the compositions and operating conditions estimated for the EHTP, even if all minor compounds are released or generated in a single puff.

Keywords : aerosol, classical nucleation theory (CNT), electrically heated tobacco product (EHTP), electrically heated tobacco system (EHTS), modeling, multicomponent, nucleation
Conference Title : ICAST 2016 : International Conference on Aerosol Science and Technology
Conference Location : Lisbon, Portugal
Conference Dates : April 14-15, 2016