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Numerical Model for the Aerosol Formation Process in an Electrically Heated Tobacco Product

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Outline

- Introduction & objective
- Modeling aerosol formation
- Simulations
- Conclusions

INTRODUCTION
&
OBJECTIVE

What is an Electrically Heated Tobacco Product (EHTP)?

Electrically Heated Tobacco System (EHTS)

(also referred to as Tobacco Heating System (THS 2.2))

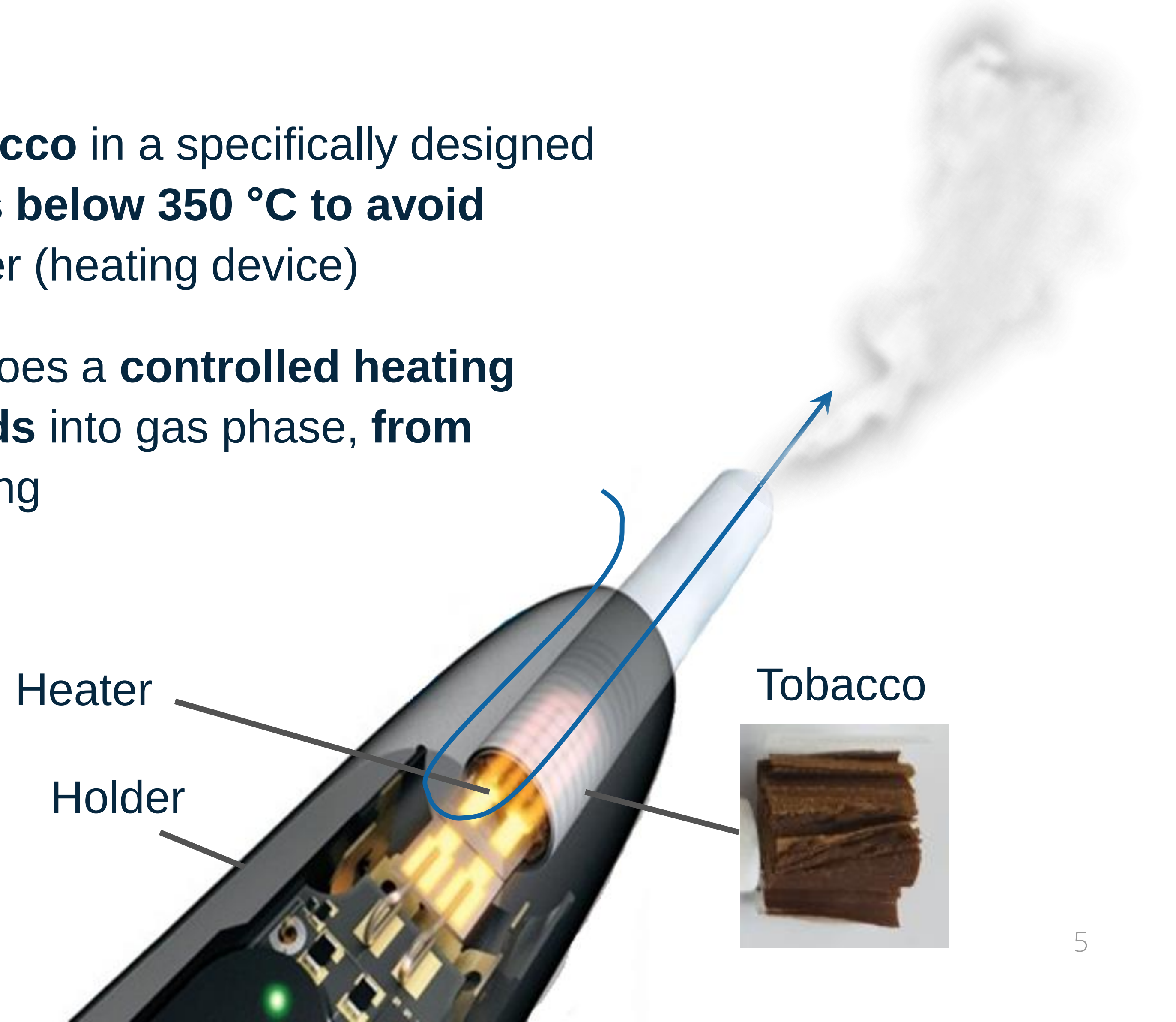
Pocket charger that is used to recharge the Holder after each use

EHTP is a novel tobacco product with unique processed tobacco made from tobacco powder

Holder into which the EHTP is inserted and which heats the tobacco material by means of an electronically controlled heater

How does EHTS function?

- During use, the **EHTS Holder heats tobacco** in a specifically designed tobacco product (EHTP) **to temperatures below 350 °C to avoid combustion** when inserted into the Holder (heating device)
- The tobacco material in the EHTP undergoes a **controlled heating process to release chemical compounds** into gas phase, **from which an aerosol is formed** during cooling



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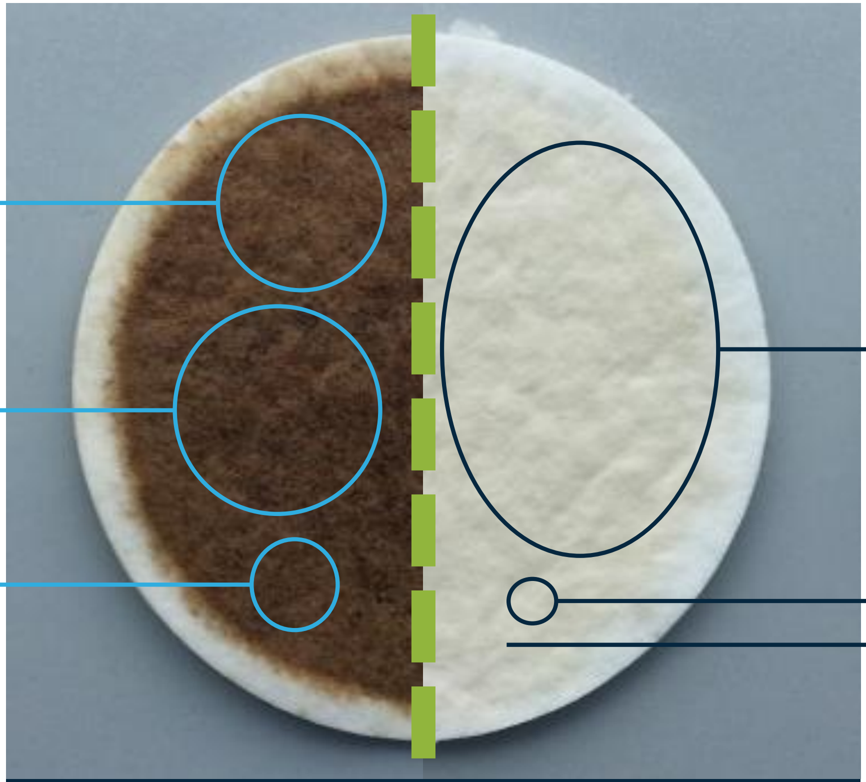
EHTS aerosol versus cigarette smoke

Cigarette smoke

Water and glycerin form 50% of smoke mass

Toxicants

Contains carbon-based solid particles



Smoke and aerosol were collected on a Cambridge filter pad using Health Canada Intense puffing regimen

EHTS aerosol

Water and glycerin form 90% of aerosol mass

Toxicants reduced by >90%

<u>No</u> carbon-based solid particles

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EHTS aerosol versus cigarette smoke

As the EHTS aerosol is very different from cigarette smoke, how is the EHTS aerosol formed?

Objective

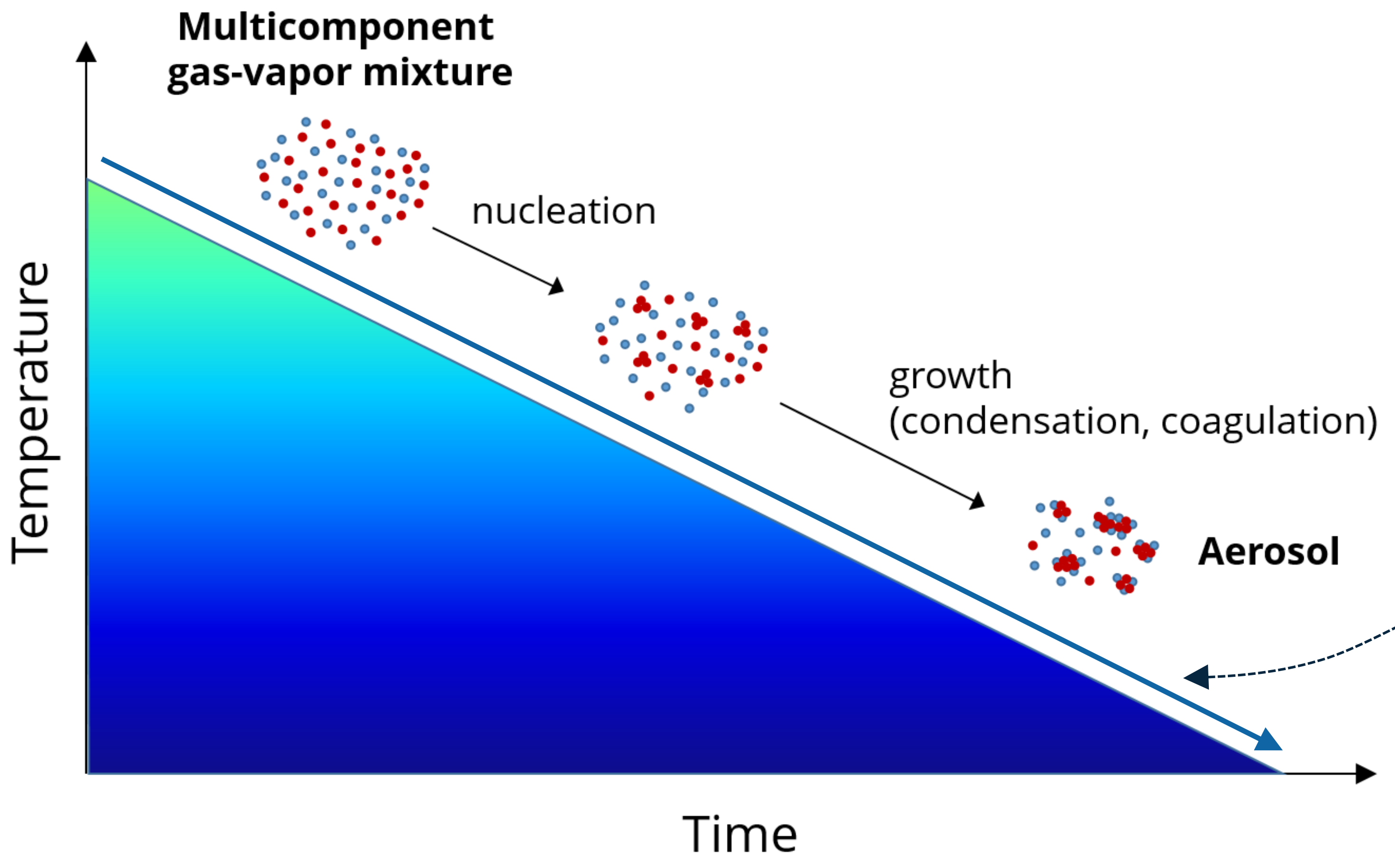
To **develop a numerical model for aerosol formation** and to use it to **investigate the role of glycerol** during aerosol formation

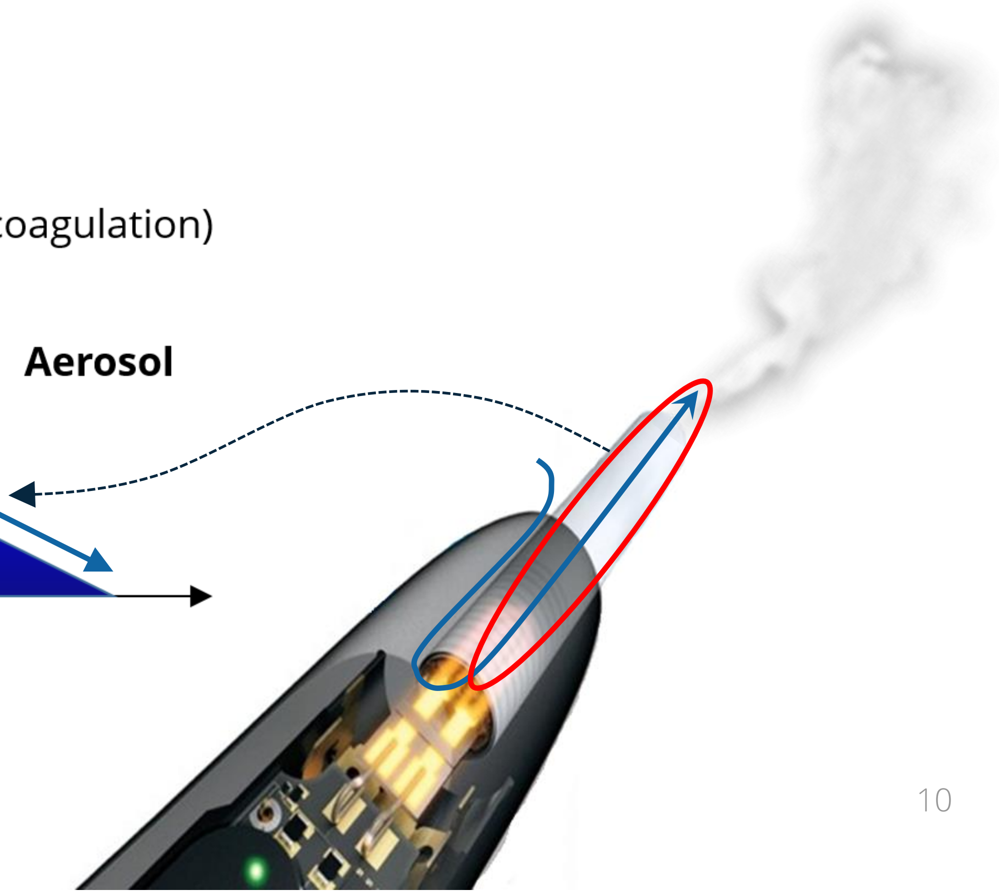
- Under realistic product operating conditions of the EHTS
- For a relevant gas-vapor mixture composition measured in the generated EHTS aerosol

and to evaluate the potential for aerosol droplet nuclei formation to happen in the absence of glycerol

MODELING AEROSOL FORMATION

Aerosol formation processes





EHTP aerosol formation modeling assumptions

- **Aerosol formation** is modeled by an **extended Classical Nucleation Theory** for multicomponent gas-vapor mixtures (Winkelmann, 2018; Frederix, 2016)
- **Eulerian-Eulerian treatment** of both gas and liquid (droplet) phases (both phases are treated as continua)
- **Multicomponent aerosol** consisting of N compounds is described by gas-vapor (Y_i) and liquid (Z_i) mass fractions and the droplet number density (M)
- **Two-moment approach** (McGraw, 1997) with a **log-normal aerosol size distribution** having fixed width (σ = 1.33)
- The fluid (gas and/or droplet) mixture density (ρ) is assumed to follow the equation-of-state of an **ideal gas mixture** with mixture compressibility ratio (Ψ)
- **Temporal evolution** only, in a **spatially homogeneous setting**

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Frederix, E.M.A. (2016) Eulerian modeling of aerosol dynamics. PhD thesis, Univ. of Twente.
McGraw, R. (1997). Aerosol Science and Technology, 27(2):255–265.
Winkelmann, C., et al. (2018). Journal of Engineering Mathematics. 108: 171-196.

Governing equations

Gas-vapor phase mass fraction equations: $$\partial_t(\rho Y_i) + S_\rho Y_i = -S_i^{nuc} + S_i^{e-c} \quad ; \quad i = 1,\ldots,N$$

Liquid phase mass fraction equations: $$\partial_t(\rho Z_i) + S_\rho Z_i = S_i^{nuc} - S_i^{e-c}; \quad i = 1,\ldots,N$$

Droplet number density equation: $$\partial_t(\rho M) + S_\rho M = J_{nuc} - J_{e-c} - J_{coa}$$

Mass fraction constraint: $$\sum_{i=1}^{N}(Y_i + Z_i) = 1$$

Equation-of-state: $$\rho = \psi(p,T)p$$

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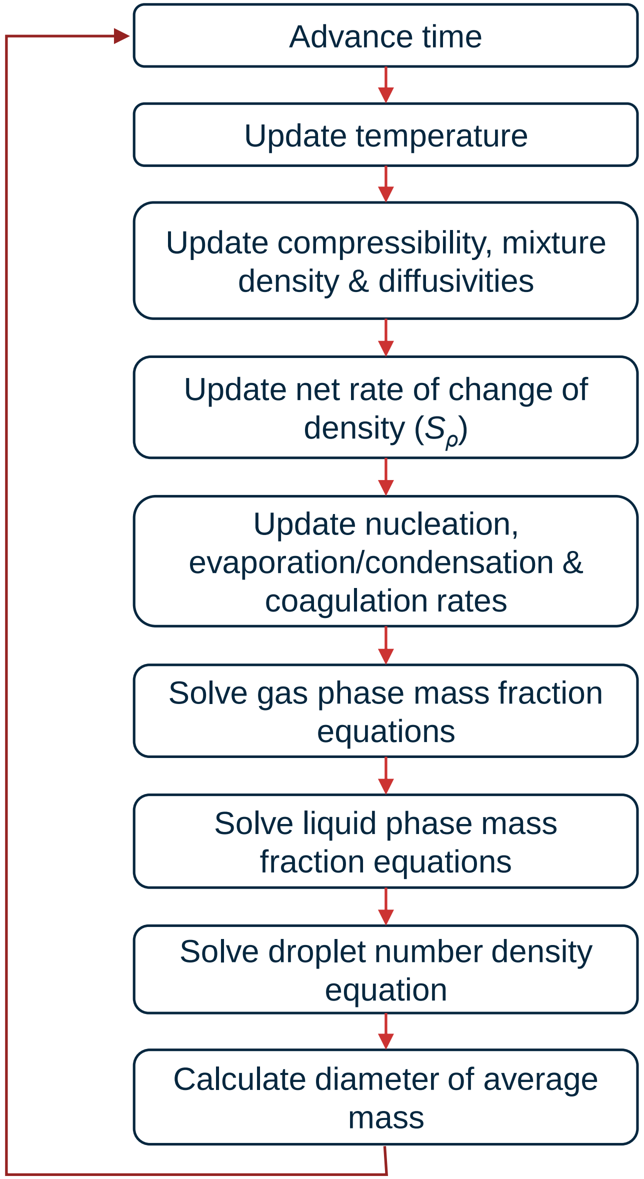
N = number of compounds i; Y_i, Z_i = gas-vapor and liquid mass fractions, respectively; M = droplet number density; ρ = fluid (gas and/or droplet) mixture density; Ψ = mixture compressibility ratio; T = temperature; p = pressure; S_ρ = net rate of change of density; t = time; S_i^{nuc}, J_{nuc} = nucleation rates; S_i^{e-c}, J_{e-c} = evaporation-condensation rates; J_{coa} = coagulation rate

Numerical algorithm

- The discretized governing equations and the models for nucleation, evaporation, condensation, and coagulation were **implemented into a segregated, finite-volume based** Computational Fluid Dynamics code using OpenFOAM® software package as described by Frederix (2016)
- **Temperature dependent** thermophysical **properties**
- The time derivative was discretized by a **second-order** implicit backward differencing **scheme**



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Frederix, E.M.A. (2016) Eulerian modeling of aerosol dynamics. PhD thesis, Univ. of Twente.

SIMULATIONS

Simulation setup

- Single computational cell
- **Constant time step** of 10^{-8} s
- The **gas-vapor mixtures were cooled down** from 623.15 K (350 °C) to 303.15 K (30 °C) **with a constant rate** of $-3 \cdot 10^5$ K/s (representative of the conditions in the EHTP) under isobaric conditions (pressure p = 101325 Pa)
- Two multicomponent **gas-vapor mixtures. Mixture A represents the EHTP aerosol composition** analytically measured by Schaller et al., (2016)

Mixture A

Mixture B

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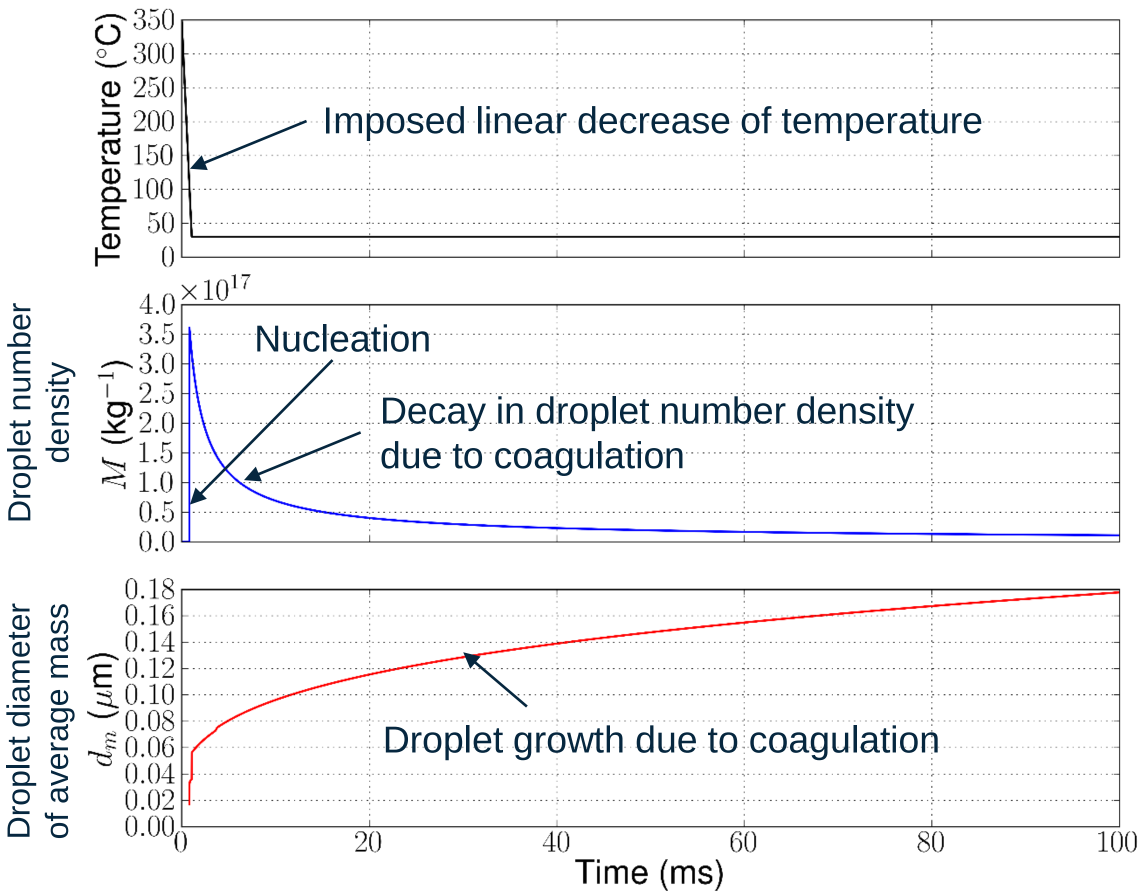
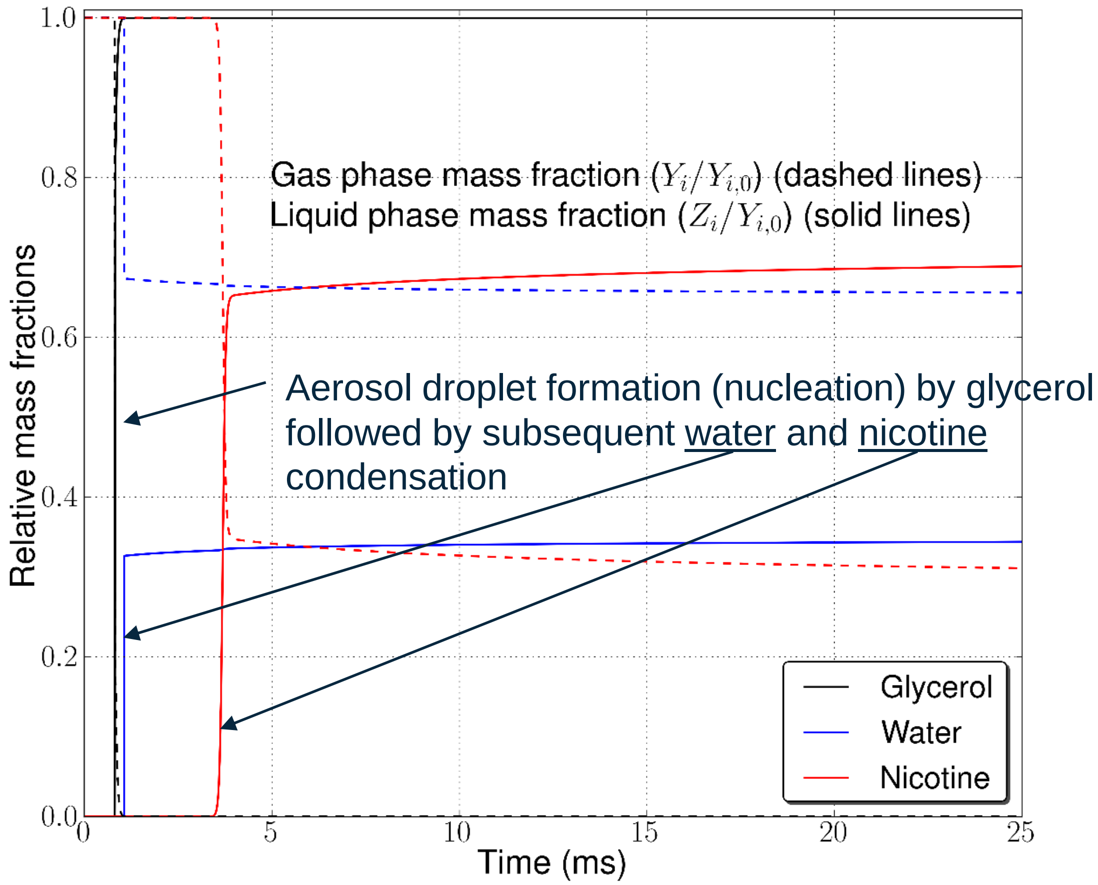
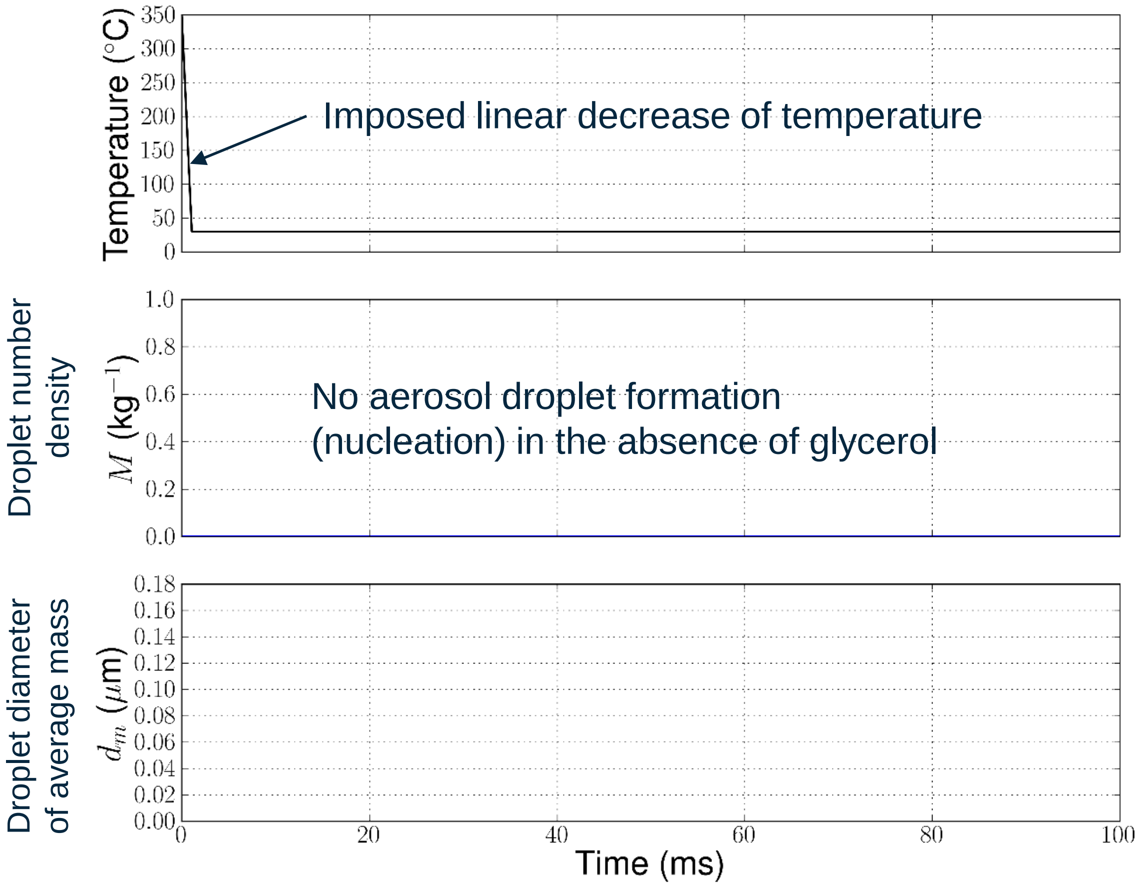
Schaller, J.-P., et al. (2016). Regulatory Toxicology and Pharmacology, 81: S48-S58.

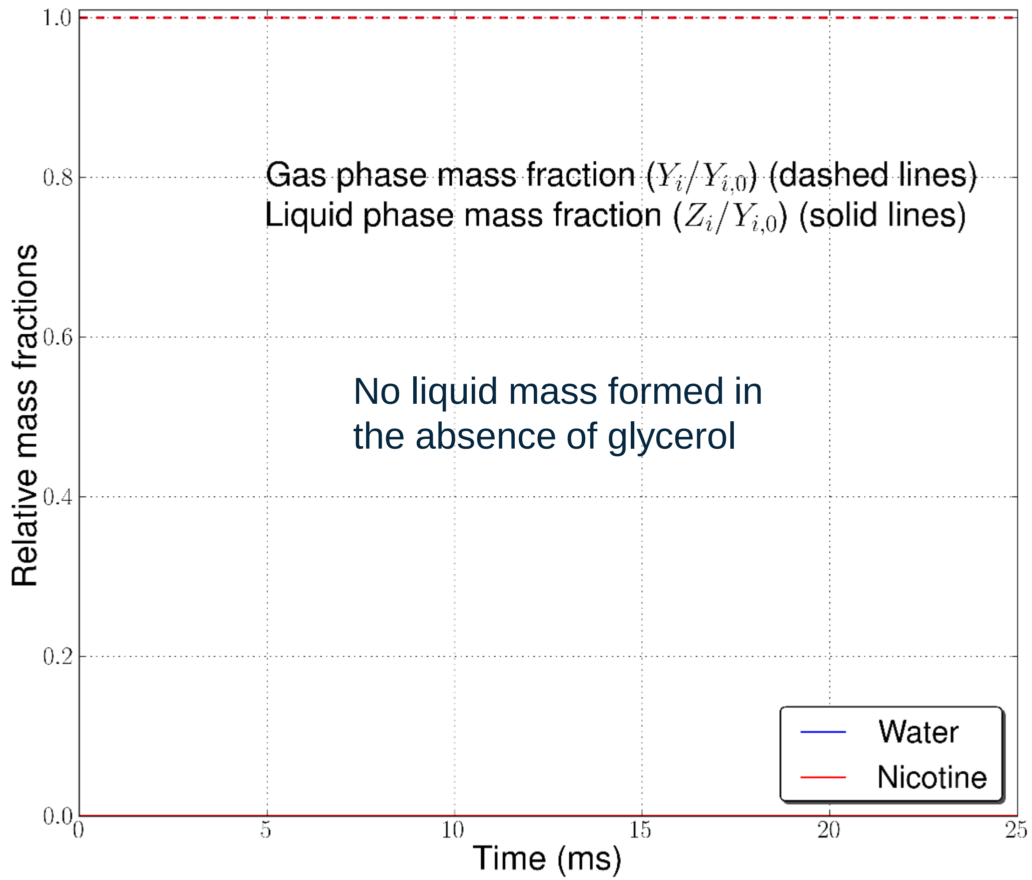
Simulation results – mixture A





Simulation results – mixture B (no glycerol)





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CONCLUSIONS

Conclusions

- According to the extended CNT, **an aerosol former, such as glycerol, is required** to be present in the gas-vapor mixture **for an aerosol to form** under the tested operating conditions of the EHTS.
- Aerosol **droplets were generated** from mixture A (representing the EHTS aerosol composition) **when the glycerol** (being evaporated from the EHTP tobacco substrate when heated) **was cooled down**.
- **Water and nicotine, were found to condensate onto the already generated droplets**, contributing to the increase of the droplet size in addition to the increase by coagulation.
- For mixture B, in which glycerol was absent, **water and other compounds in the gas-vapor mixture were not able to reach supersaturation** and could therefore not generate aerosol droplets from the multicomponent gas-vapor mixture at the tested operating conditions of the EHTS.

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Thank you for your attention!

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