Predicting Supersaturation in a Laminar Flow

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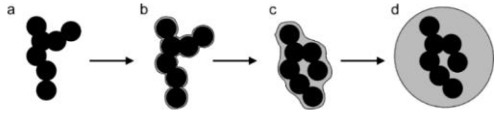
Background

- Condensation is a major aging pathway for atmospheric aerosols
- Aging alters their climate forcing properties
- Saturator + condenser is a common laboratory technique for simulating condensational aerosol aging



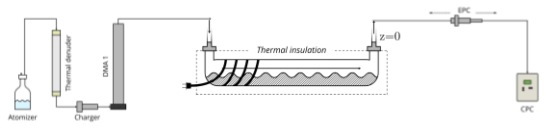
Soot aggregate acquiring coating and restructuring

Project goal

- In a related project, we are studying experimentally condensation of different vapors on soot. Supersaturation is needed to calculate the amount of condensate.
- The goal of this project was to accurately predict how much material would condense on particles knowing saturator and condenser temperatures

Experimental setup

- Aerosol was generated, size-classified, passed through a saturator, condenser, and size was measured at different distances after the saturator
- An Electrostatic Particle Classifier (EPC) was initially installed immediately after the saturator. Then more and more tubing was added before the EPC to measure particle size as a function of distance



Aerosol growth measurement system

Modeling of particle growth

- Rate of growth of spherical particles depends on ambient vapor concentration and temperature (Seinfeld & Pandis, 2016)

$$\frac{dR_p}{dt} = \left(C - C_{s,Kelvin}\right) C_{FS} D_i M \frac{1}{\rho R_p}$$

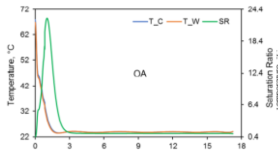
- Vapor concentration as a function of particle position in the condenser needs to be determined to calculate growth

1D model

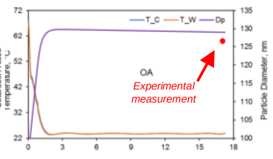
- Chen et al., 2018 used a 1D model to calculate vapor concentration and supersaturation (ζ)
- The model is primed with wall and centerline temperatures and assumes vapor is distributed uniformly across the tube

$$\frac{dC}{dt} = -4\pi n R_p D_i C_{FS}\left(C - C_{s,Kelvin}\right) - k_d\left(C - C_{wall}\right)$$

$$k_d = \frac{3.65 D_i}{R^2}$$



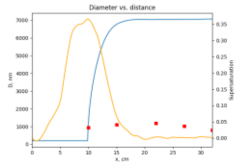
Saturation ratio, oleic acid



Particle diameter, 100 nm PSL

Failure of 1D model

- The 1D Model significantly overestimated particle growth and vapor supersaturation with water
- Attempts were made to improve the model:
  - Delayed start time for growth with water vapor (to account for hydrophobicity of soot)
  - Latent heat released by condensing water
  - Changing flow velocity due to cooling and loss of mass
- Possible reasons why closure between experiments and model wasn't attained:
  - The model relies on experimentally obtained gas temperature, which is hard to measure in a 5 mm ID tube
  - Temperature and concentration are not evenly distributed radially in a laminar flow



Water condensing on 240 nm soot, saturator at 80 ° C

2D model

- Heat conduction and mass diffusion are modelled by solving two partial differential equations:

$$\frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T = \alpha_t \nabla^2 T$$

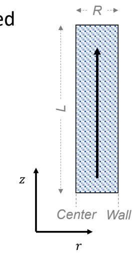
$$\frac{\partial C}{\partial t} + \vec{v} \cdot \nabla C = D_i \nabla^2 C$$

- The model is primed with wall temperature. Saturated vapor near the wall is assumed.
- For steady-state, laminar flow in cylindrical coordinates:

$$\frac{\partial T}{\partial z}\left[1 - \frac{r^2}{R^2}\right] U = \alpha_t \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r}\right)$$

$$\frac{\partial C}{\partial z}\left[1 - \frac{r^2}{R^2}\right] U = D_i \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial C}{\partial r}\right)$$

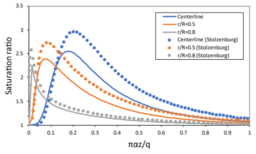
- Finite element method was used to solve the PDEs



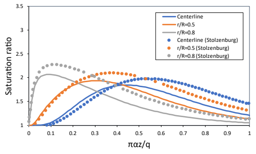
Spatial domain

Model verification

- The model has been verified against Hering & Stolzenburg, 2005
- The slight mismatch between absolute values was likely caused by the authors using a different Antoine equation (not reported in the paper)

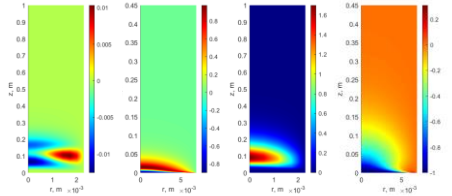


Cold-to-hot transition



Hot-to-cold transition

Modeled supersaturation



Water hot → cold (exit)	Water cold → hot (entrance)	TEG hot → cold (exit)	TEG cold → hot (entrance)

What determines the difference in supersaturation location?

- Behavior of supersaturation depends on Lewis number (Le)

$$Le = \frac{\alpha_T}{D_i}$$

$$\alpha_T = \frac{k}{\rho C_p} \text{ (thermal diffusivity)}$$

- Lewis number depends on condensing material and diffusion medium (air in our case)

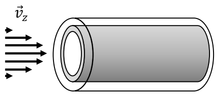
Triethylene Glycol ($Le > 1$)	Water ($Le < 1$)
Supersaturation is higher	Supersaturation is lower
Supersaturation occurs mostly at hot → cold transition	Supersaturation occurs mostly at cold → hot transition

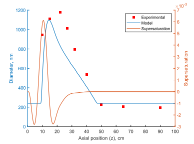
Modeled vs. measured particle growth

- Growth was calculated assuming even mass distribution over equal-width concentric shells and non-mixing layers
- Let N be the total number of shells

$$D = \frac{1}{N^2} \sum_{n=1}^{N} D_n (2n - 1)$$

- D is the mean particle diameter at position z





Sample growth curve, 240 nm soot, water

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