Computational Tool for Estimating Indoor Aerosol/Vapor Concentration

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Questions related to Second Hand Exposure from E-Cigarettes*

- What chemicals are potentially delivered to non-users?
- How exhaled aerosol properties impact exposure?
- How far aerosol can travel in a confined space?
- What is aerosol level in different space settings?

* Source: FDA Public Workshop - Electronic Cigarettes and the Public Health, June 1-2, 2015, http://www.fda.gov/TobaccoProducts/NewsEvents/ucm439029.htm

Outline

- Model development
- Comparison of model predictions with experimental data
  - Exhaled aerosol released into a room (ALCS study)
  - Smoking-machine generated aerosol released into a room (published literature data)
- Examples of model applications
  - Usage variability
  - Room ventilation effects
- Model enhancement

Two Types of Computational Models

Well-mixed Model

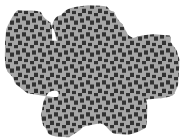
- Total, vapor and particulate concentrations of each constituent in air
- Average values for the entire space as a function of time

Distributed Model

- Total, vapor and particulate concentrations of each constituent in air
- Spatial and temporal distribution inside the space

The focus of this talk is on the Well-mixed model

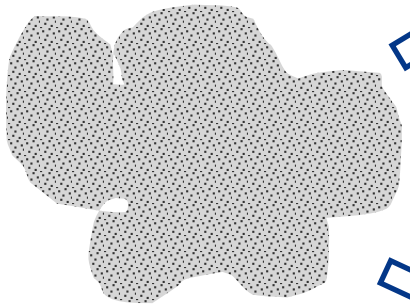
Physical and Mathematical Bases of Model (First Principle Approach)



Aerosol exhaled by e-cigarette users into indoor space

Mixing with room and ventilation air

Dilution/ Evaporation



Low Concentration (mostly in vapor phase)

Carried out by vent air

Inhaled by occupants

Remains airborne indoor

Deposits on surfaces

Conservation of Mass*

$$m_{vi} + m_{li} = m_{i,source}$$

Vapor/Liquid Partitioning

$$\frac{m_{vi}}{m_{li}} = \frac{a_i M}{\sum_j m_{l,j}}, a_i = \frac{(\gamma x P_{sat})_i V_a}{RT}$$

Mixing / Dilution

$$V_{room}\frac{dC_i(t)}{dt} = \frac{dm_{i,source}}{dt} - Q_a C_i(t)$$

Air flow and species transport equations

* Notations are given in the addendum

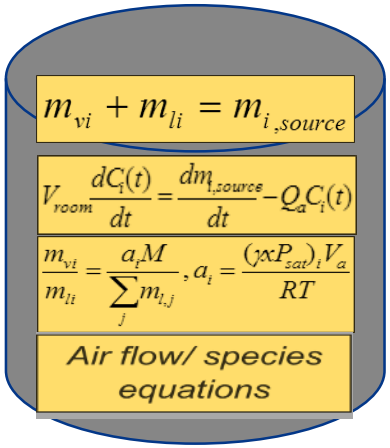
Model Functionality

INPUTS

Measured Exhaled Aerosol

Space Size

Air Change Rate



OUTPUTS

Carried out by vent air

Inhaled by occupants → **Secondhand Exposure**

Remains airborne indoor

Deposits on surfaces → **Thirdhand Exposure**

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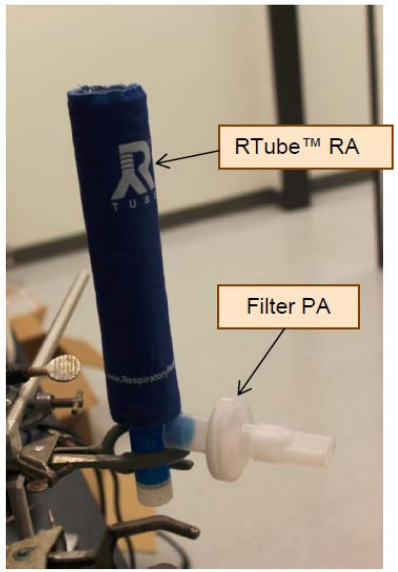
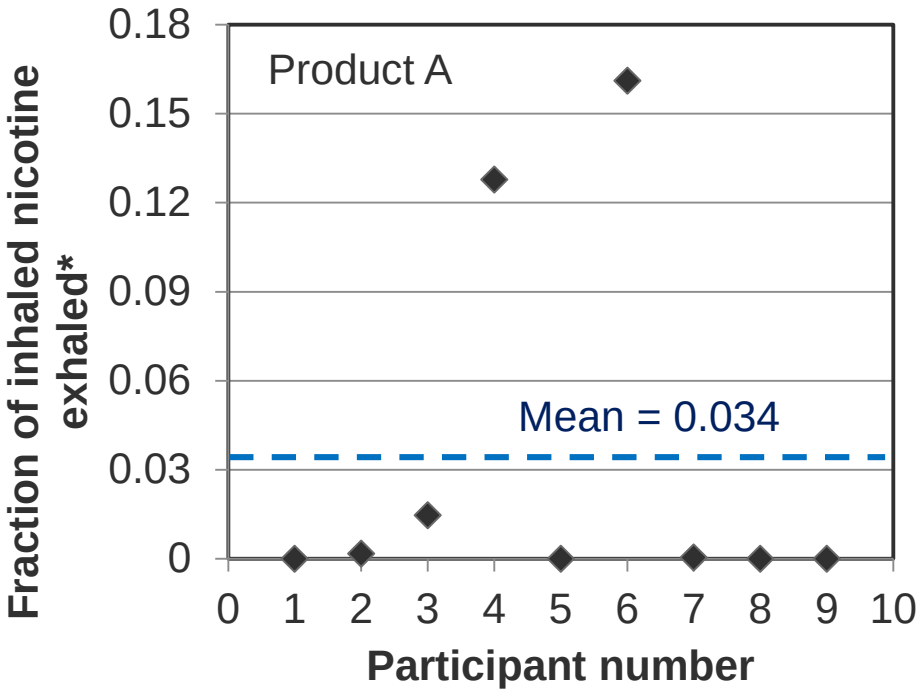
Model Input Data: Exhaled Aerosol



Exhaled Breath Condensate



9 participants used product A ; 10 puffs, 5s duration; exhaled aerosol collected into EBC system after each puff; analyzed for nicotine and other constituents.

Product A: Prototype E-cigarette (GS)

- Liquid composition: PG/Gly/Water/Nic (W%): 41/42/14.6/2.4
- Aerosol mass: 5.1 mg per puff @ 55 cc/ 5 s

* Estimated assuming 5.1 mg of aerosol is inhaled in each puff

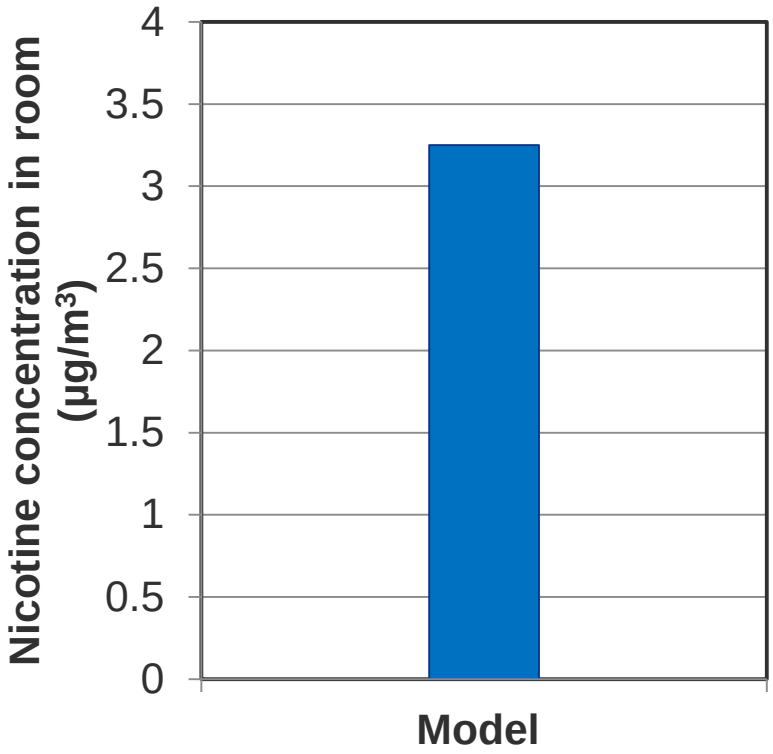
Room Concentration Due to Exhaled Aerosol*

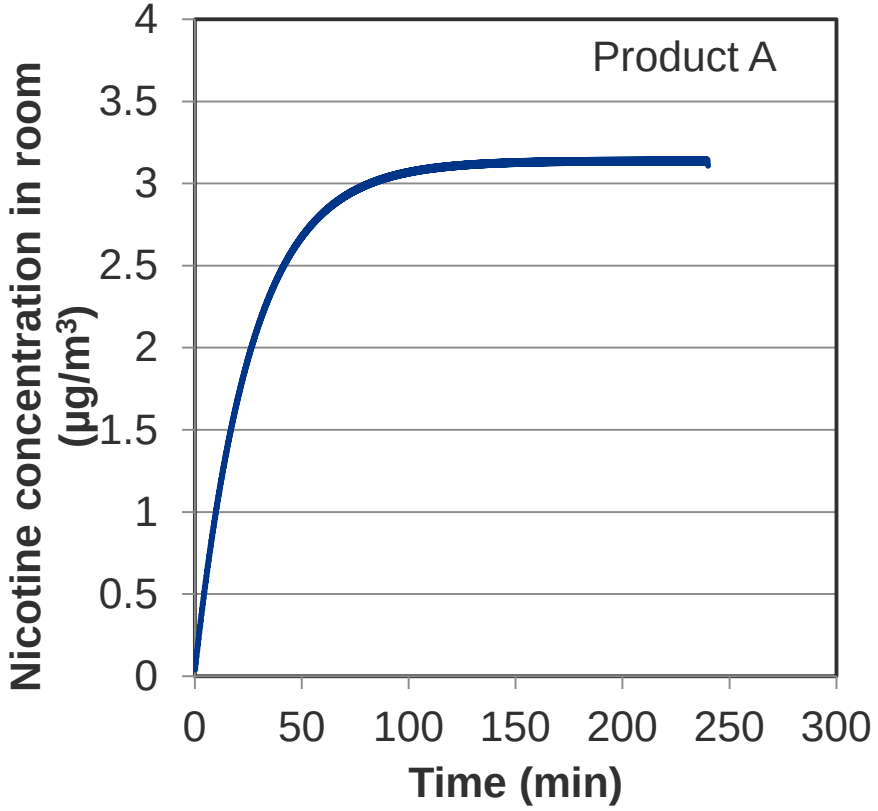
- Mobile experimental chamber (112 m^3), conditioned space with fixed ventilation (2.25 ACH)
- Same 9 participants used same product at a prescribed usage conditions (10 puffs, 5s puff duration, every 30 min, over 4 hour)
- Room level of constituents measured over a 4 h period.

* M. Sarkar et. al. “Are Chemical Constituents Exhaled in a Room Where e-Vapor Products are Used?, presented at 69th Tobacco Science Research Conference, September 20-23, 2015.

Model Predictions: Room Concentration

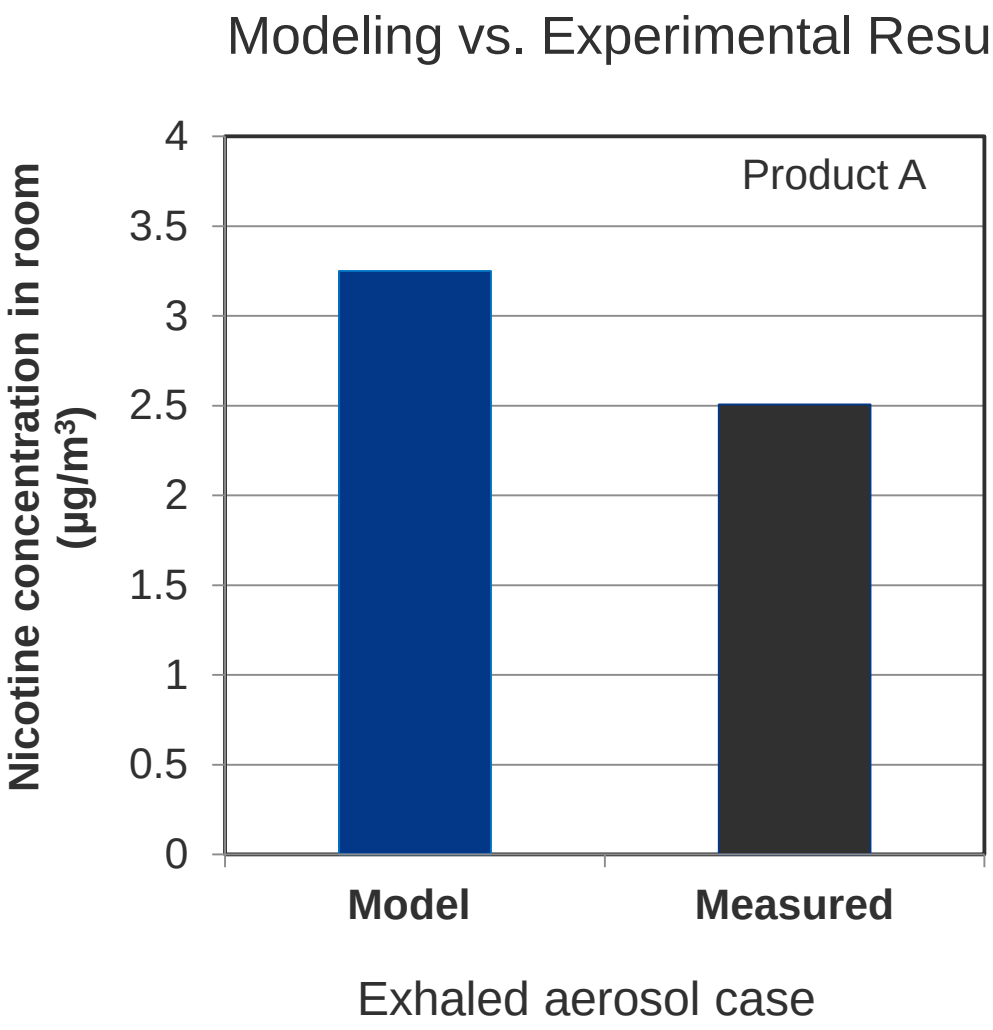
Modeling Results: Room concentration after 4 hours



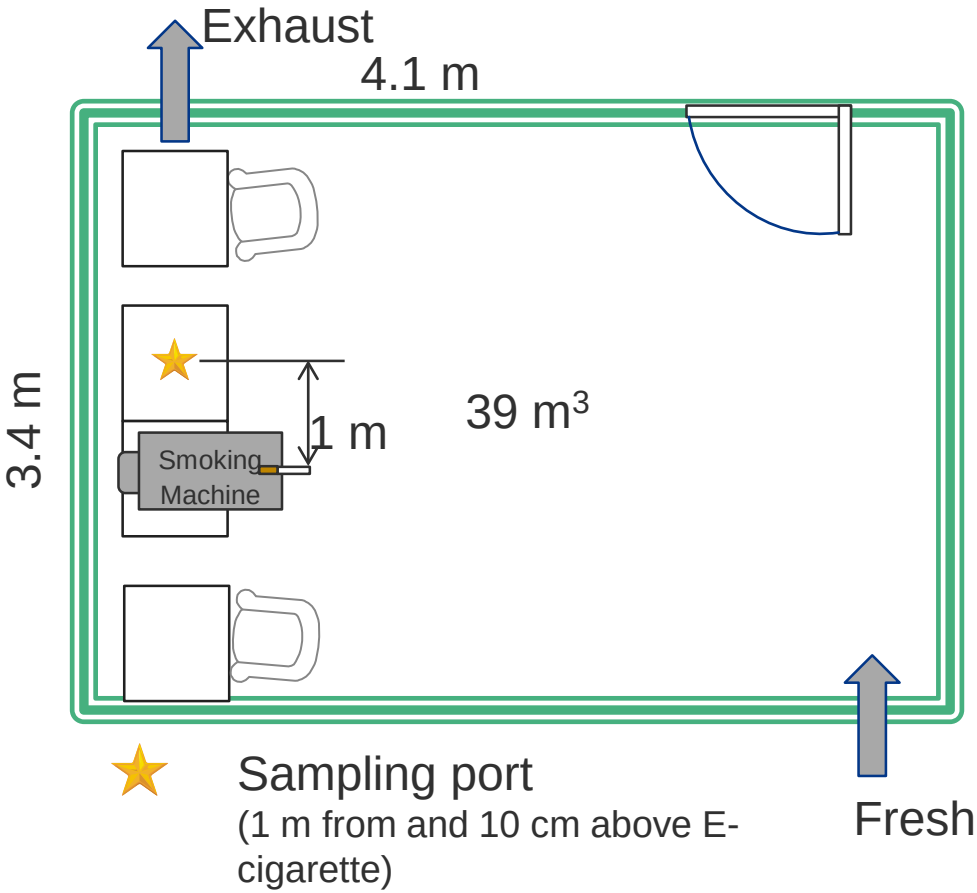


Exhaled aerosol case

Model vs. Experimental Data: Room Concentration



Model Input Data: Smoking Machine Case*

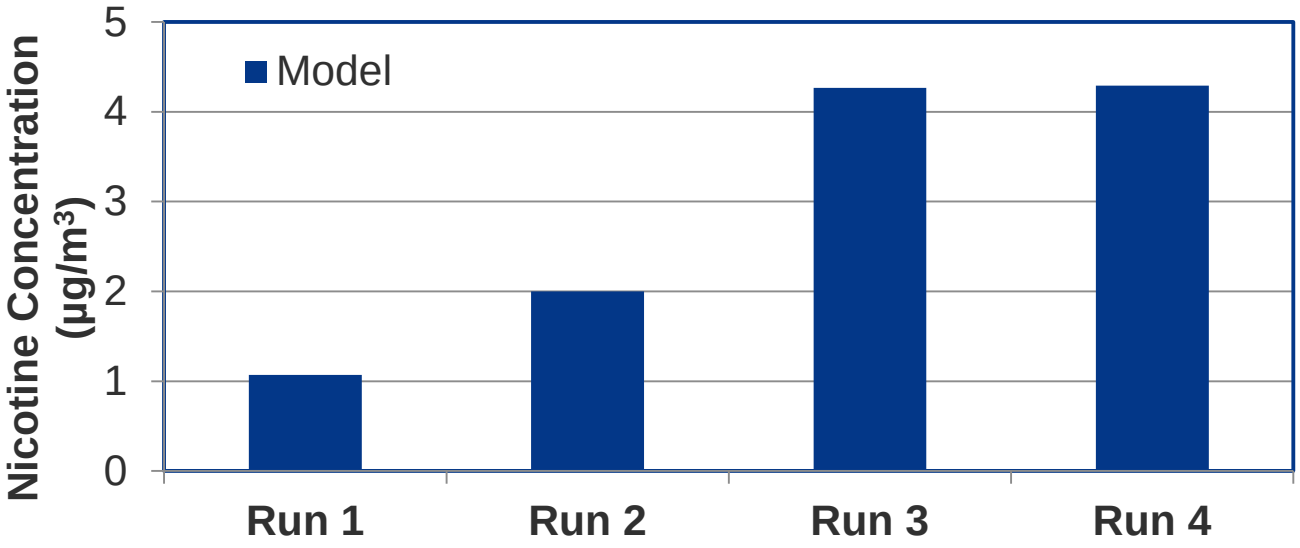


- Aerosol released twice at 30 minute apart during a 60 min period.
- 70 ml puff, 1.8 s duration, 10 s between puffs
- Nicotine and other concentrations in room over 60 min after first release were measured

Locations of equipment and fans do not correspond to actual setting (not known)

* Czogala et al. (2014), Secondhand exposure to vapors from electronic cigarettes, Nicotine and Tobacco Res, *16 (6): 655-662*

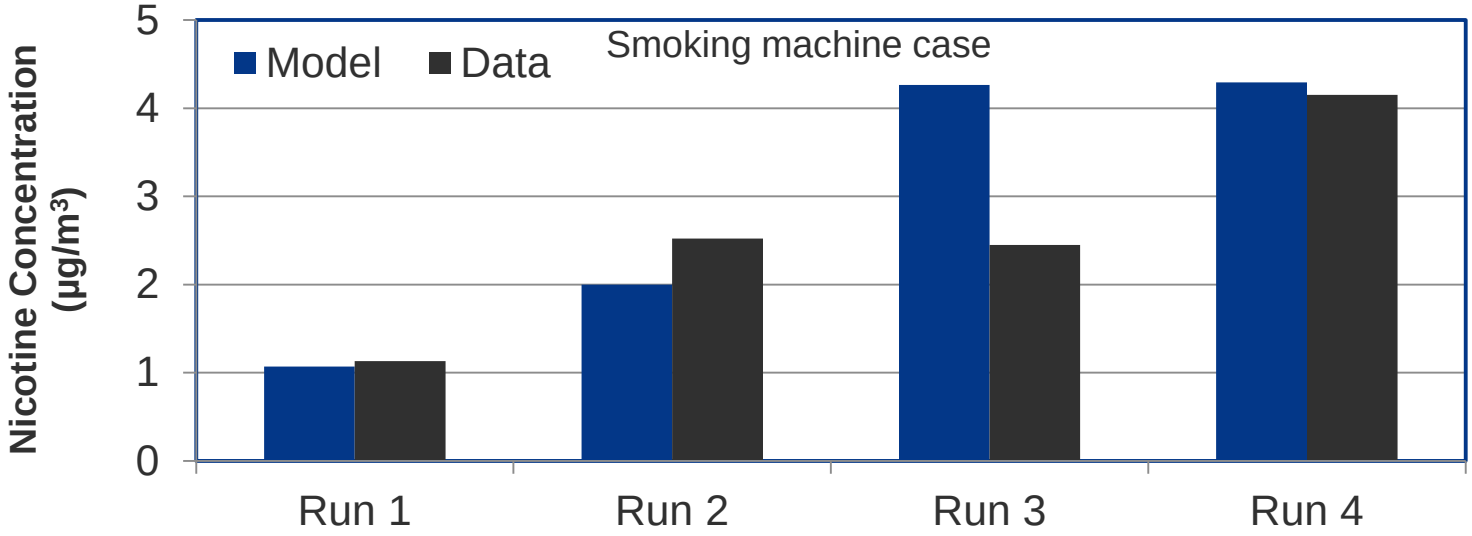
Modeling Results: Smoking Machine Case



Runs	Nic.% in formulation	Aerosol Release	Ventilation (ACH)
Run 1	1.8 (EC2)	Low (7 puffs)	9.86
Run 2	1.8 (EC2)	Low (7 puffs)	6.81
Run 3	1.8 (EC2)	High (15 puffs)	6.83
Run 4	1.8 (EC2)	High (15 puffs)	6.8

Model predicts the trend successfully

Model Results vs Experimental Data*



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*Everything being comparable, nicotine concentrations in the room for Runs 3 and 4 are expected to be comparable. The observed difference may be due to measurement variability.

Modeling predictions align well with experimental observations

* Data from Czogala et al. (2014), Secondhand exposure to vapors from electronic cigarettes, Nicotine and Tobacco Res, *16 (6): 655-662*

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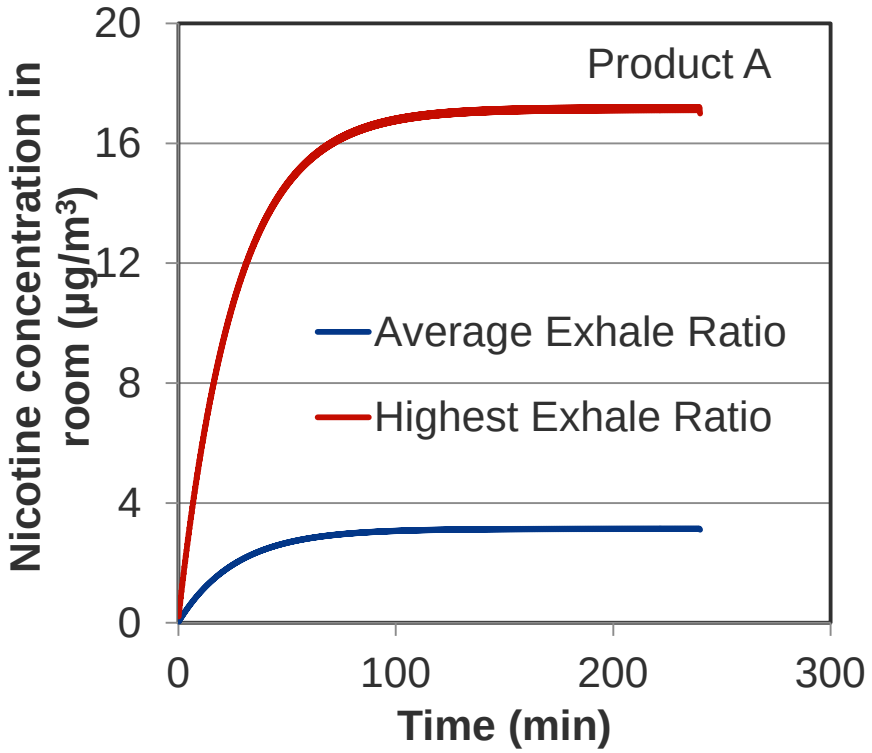
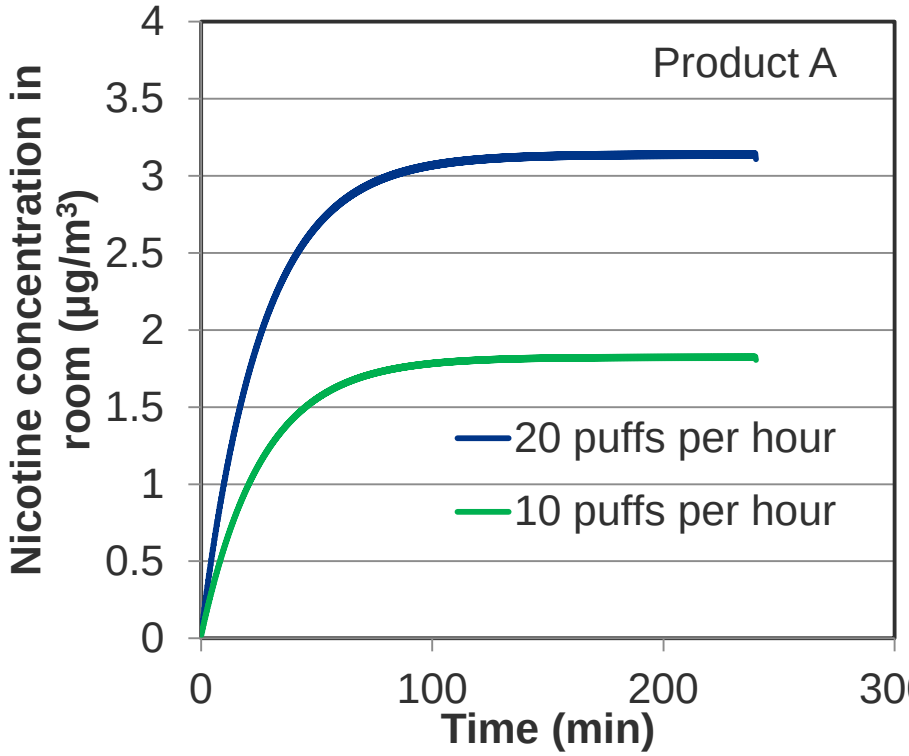
Example Scenario 1: Usage Variability

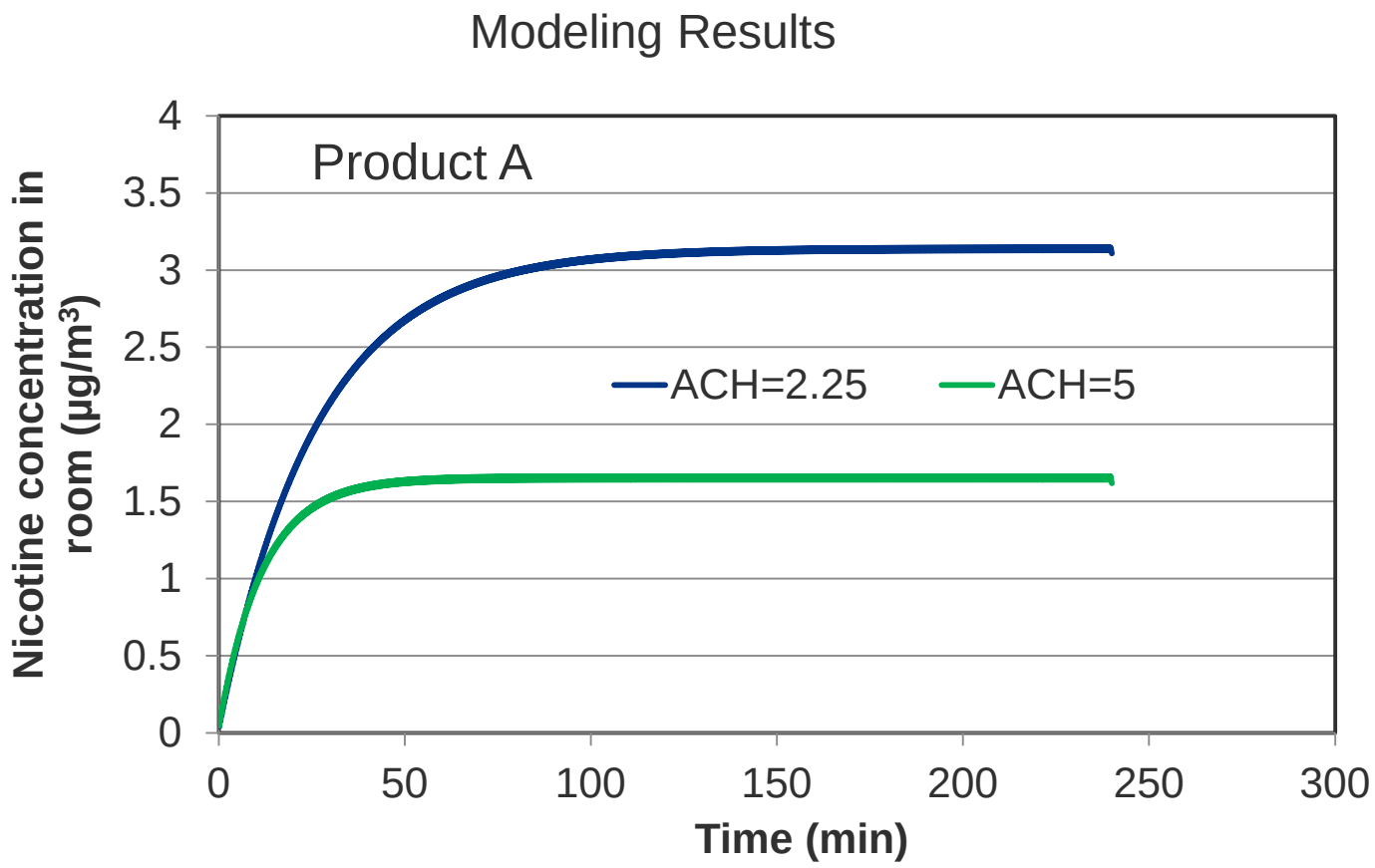
Modeling Results





Individual usage variability can be evaluated

Example Scenario 2: Room Ventilation Effects



Effects of space size and ventilation rate can be estimated

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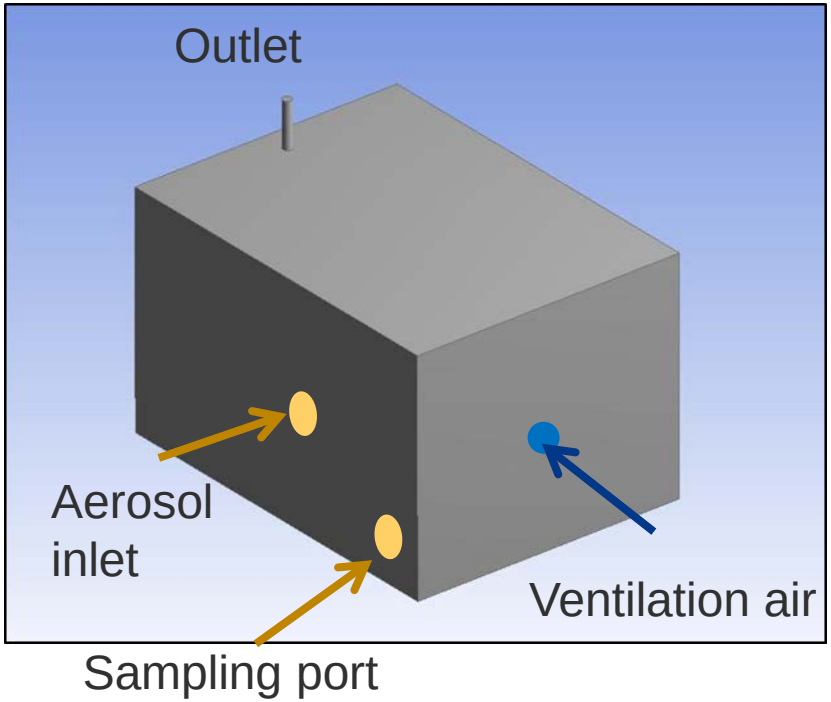
Distributed Model

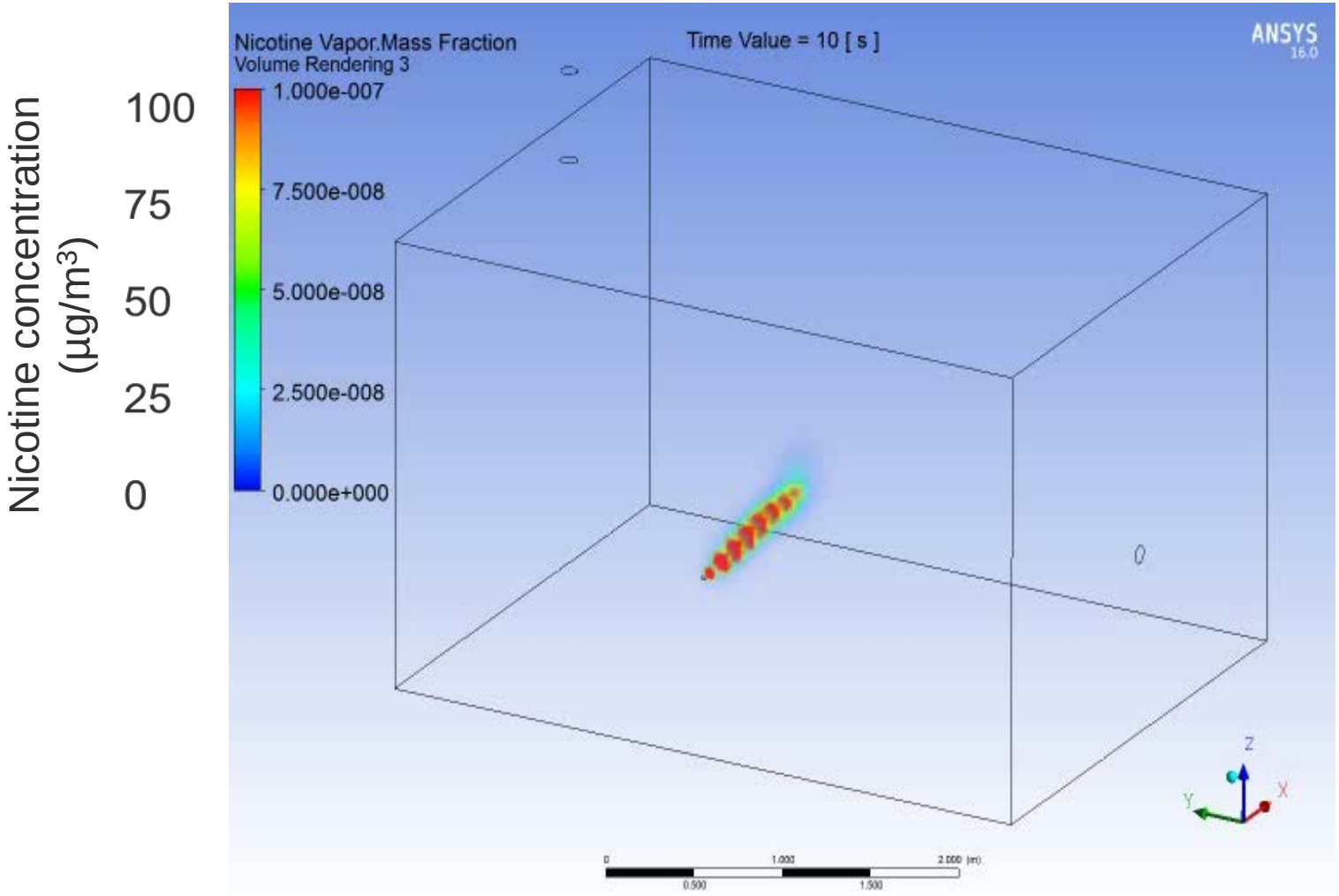
- Chamber volume = 30 m^3
- Air change rate = 0.5 per hour
- Aerosol from smoking machine
- 6 series of 13 puffs, 5 min apart, over 70 minutes
- 2.7 mg aerosol/puff



Data from:

Otmar Geiss, Ivana Bianchi, Francisco Barahona, Josefa Barrero-Moreno, Characterisation of mainstream and passive vapours emitted by selected electronic cigarettes, International Journal of Hygiene and Environmental Health 218 (2015) 169–180.

Example of Distributed Model Result*



*A modeling scenario based on input data described in: Otmar Geiss, Ivana Bianchi, Francisco Barahona, Josefa Barrero-Moreno, Characterisation of mainstream and passive vapours emitted by selected electronic cigarettes, International Journal of Hygiene and Environmental Health 218 (2015) 169–180.

Summary

- Developed computational models using principles similar to those referenced by EPA for indoor air quality analysis
- Validating models using data from controlled studies with e-cigarette products
- Apply models to:
  - Address types of questions listed earlier
  - Run simulations for multiple scenarios to evaluate the impacts of individual user variability, indoor space size, air change, number of occupants, etc.
- Improve models as additional data become available
- Publish the work in a peer-reviewed journal

http://www.altria.com/alcs-science

Thank You

Addendum: Notations for Equations

m_{vi}	*mass of vapor phase*
m_{li}	*mass of liquid phase*
m_i	*total mass, constituent i*
M	*molecular mass*
γ	*activity coefficient*
x	*mole fraction*
P_{sat}	*saturation pressure*
T	*temperature*
R	*universal gas constant*
V	*air or room volume*
C	*concentration of i*
Q	*ventilation air rate*
t	*time*

Conservation of Mass*

$$m_{vi} + m_{li} = m_{i,source}$$

Vapor Liquid Partitioning

$$\frac{m_{vi}}{m_{li}} = \frac{a_i M}{\sum_j m_{l,j}}, a_i = \frac{(\gamma x P_{sat})_i V_a}{RT}$$

Dilution

$$V_{room} \frac{dC_i(t)}{dt} = \frac{dm_{i,source}}{dt} - Q_a C_i(t)$$