A Distributed Computational Fluid Dynamics (CFD) Model for Estimation of Room Air Levels of Selected Aerosol Chemicals from Emission of E-Vapor Products (EVP)

Ali A. Rostami[1], *Samuel A. Agyemang*[2] *and Yezdi B. Pithawalla*[1]

[1] Altria Client Services LLC, Research Development & Regulatory Affairs, Richmond, Virginia, USA

[2] TriMech Solutions LLC , Glen Allen, Virginia , USA

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CORESTA Congress, October 9-13, 2016, Berlin, Germany

Health Effects of E-Cigarettes on Non-Users

FDA has expressed interest in understanding:

- What chemicals are potentially delivered to nonusers?
- How do exhaled aerosol properties impact potential secondhand exposures?
- How far can aerosols travel in a confined environment?
- What is aerosol level in different space settings such as cars, homes, office and public buildings?

Proposed Approach

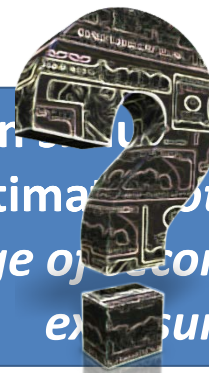
Combination of controlled clinical studies & computational modeling

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

Approach: Exposure Assessment of Secondhand Exposure from Vaping

Controlled Clinical Study: Measure room air levels of selected constituents

Develop Computational Models



Run [illegible] ons to estima[illegible] *otential range o[illegible] cond-hand ex[illegible] sure*

Exposure assessment of secondhand aerosol from e-cigarettes

- **Individual user variability**
- **Number of occupants**
- **Space settings: Homes, cars, etc.**
- **Size, ventilation, etc.**

*M. Sarkar et. al. "Are Chemical Constituents Exhaled in a Room where e-vapor products are used?". Presented at 69th Tobacco Science Research Conference, Sept. 20-23, 2015.
*A Rostami et. al. "Computational Tool for Estimating Indoor Aerosol/Vapor Concentration ". Presented at 69th Tobacco Science Research Conference, Sept. 20-23, 2015.

Two Types of Computational Models Developed at ALCS*

Models based on principles similar to those used in the indoor air quality assessment models, referred to by the EPA**

Well-mixed Model

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

Rostami et al., A well-mixed computational model for estimating room air levels of selected constituents from e-vapor product use, ***Int. J. Environ. Res. Public Health*, *August 2016.***

Distributed CFD Model

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

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*Altria Client Services LLC, **https://www.epa.gov/ttn/scram/aqmindex.htm

Physical and Mathematical Bases of Model

Exhaled E-cigarette Aerosol Particles

Mix with room air

Evaporation

Vapors

Exit through vent

Remains airborne (Secondhand exposure)

Deposits on surfaces (Thirdhand exposure)

Energy Conservation Equation

$$\frac{\partial(\rho c_p T)}{\partial t} + \frac{\partial(\rho c_p u_j T)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(k + \frac{\rho c_p \nu_T}{Pr_T}\right)\frac{\partial T}{\partial x_j}\right] + \frac{\partial}{\partial x_j}\left[\sum_{i=1}^{4} h_i \rho \left(D_i + \frac{\nu_T}{Sc_T}\right)\frac{\partial Y_i}{\partial x_j}\right] + S^{(E)}$$

Species Transport Equation

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j Y_i) = \frac{\partial}{\partial x_j}\left[\rho\left(D_i + \frac{\nu_T}{Sc_T}\right)\frac{\partial Y_i}{\partial x_j}\right] + S_i^{(Y)}$$

Notations are given in the addendum

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Physical and Mathematical Bases of Model

Particle Transport Equation

$$\frac{d}{dt}(m_p u_p) = F^D + F^L + F^{BM} + F^G$$

$$\frac{dm_p}{dt} = -\sum_{i=1}^{4} \pi d_p^2 J_i$$

Thermodynamic Relations

$$H_i = A_i\left(1 - \frac{T}{T_{c,i}}\right)^{n_i}$$

$$Log_{10}P_{sat,i} = A_i + \frac{B_i}{T_p} + C_i\, Log_{10}T + D_i T + E_i T^2$$

Other Equations in Model

- Mass Conservation/Continuity Equation
- Momentum Conservation Equation
- Turbulence Models (Realizable k-ε)
- User Defined Functions (UDF's)

Model Development Platform:
ANSYS® Fluent 17.0 Computational Fluid Dynamics Software

Notations are given in the addendum

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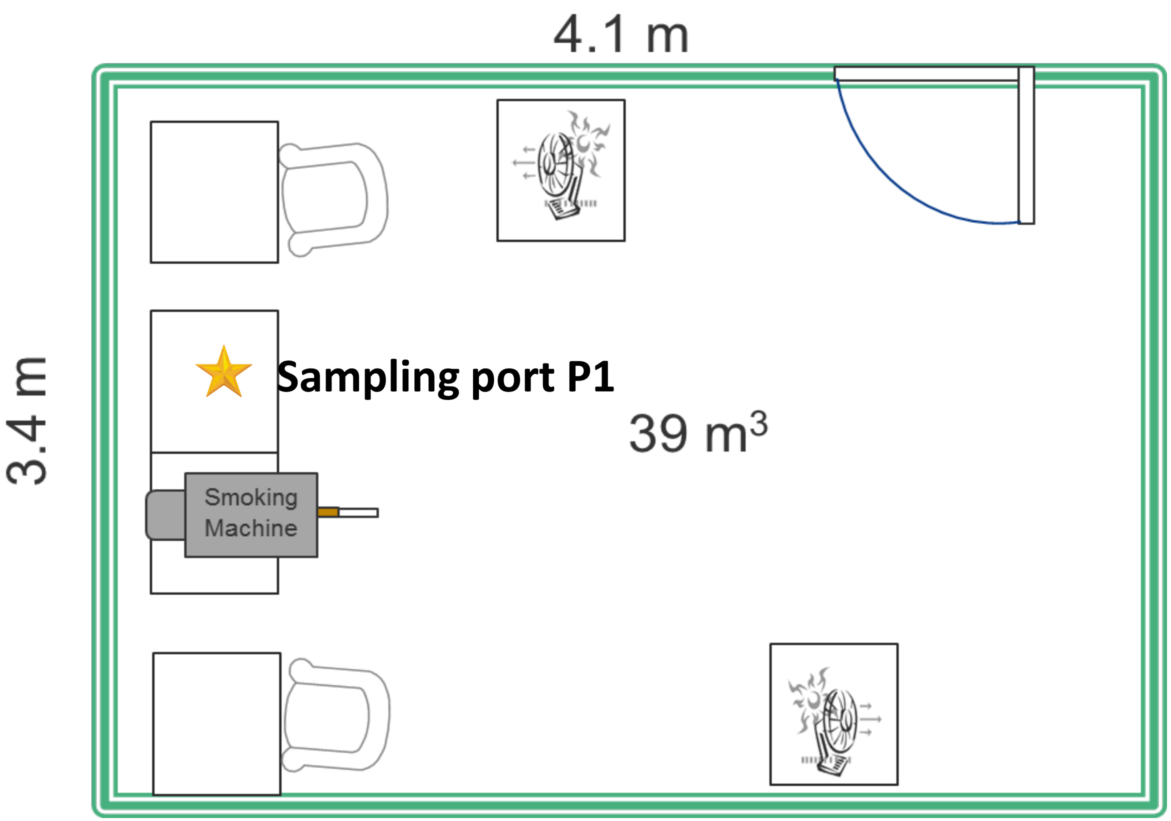
Model Validation: Smoking Machine Case[1]



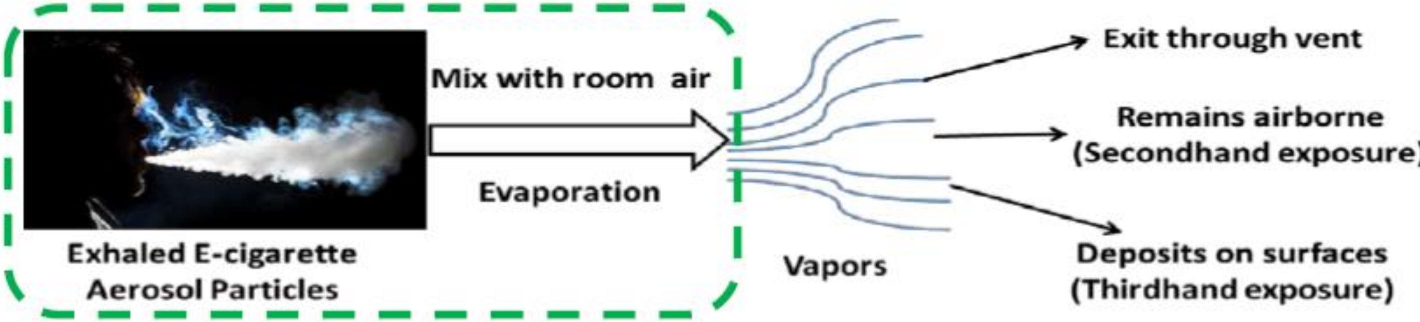
- Two doses of aerosols from e-cigarettes are released into the room at 30 minutes apart
- Each dose is either 15 (high) or 7 (low) puffs
- Ventilation levels (high ~ 10 ACH, low ~7 ACH)

Locations of equipment and fans are estimated (actual setting not known)

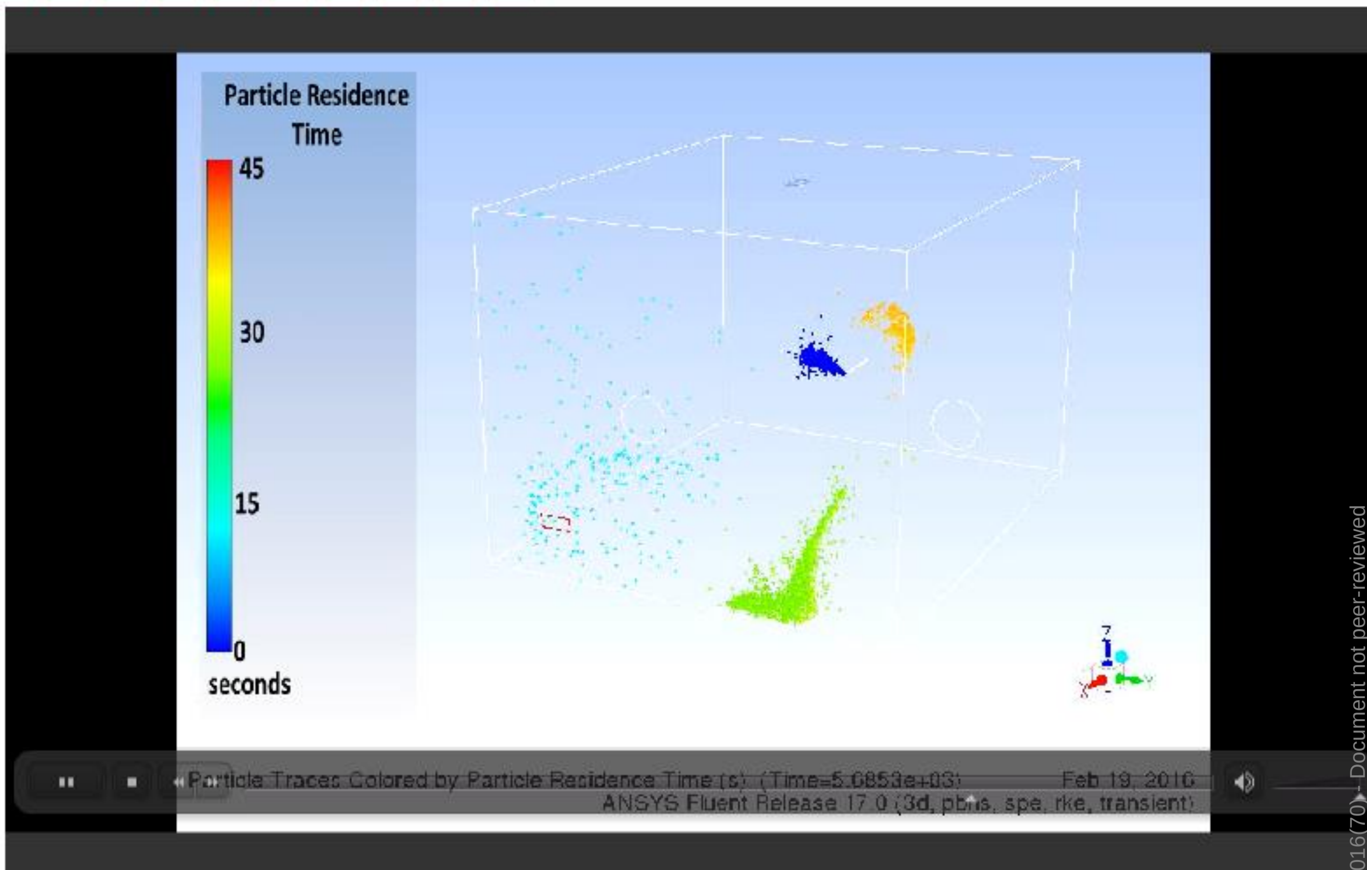
[1]Czogala et al. (2014), Secondhand exposure to vapors from electronic cigarettes, Nicotine and Tobacco Res, *16 (6): 655-662.*

ACH = Air Change per Hour

Room Aerosol Circulation Profile

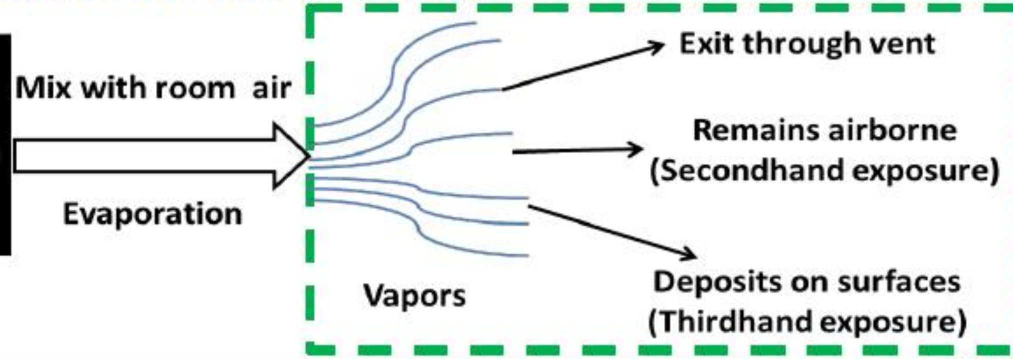


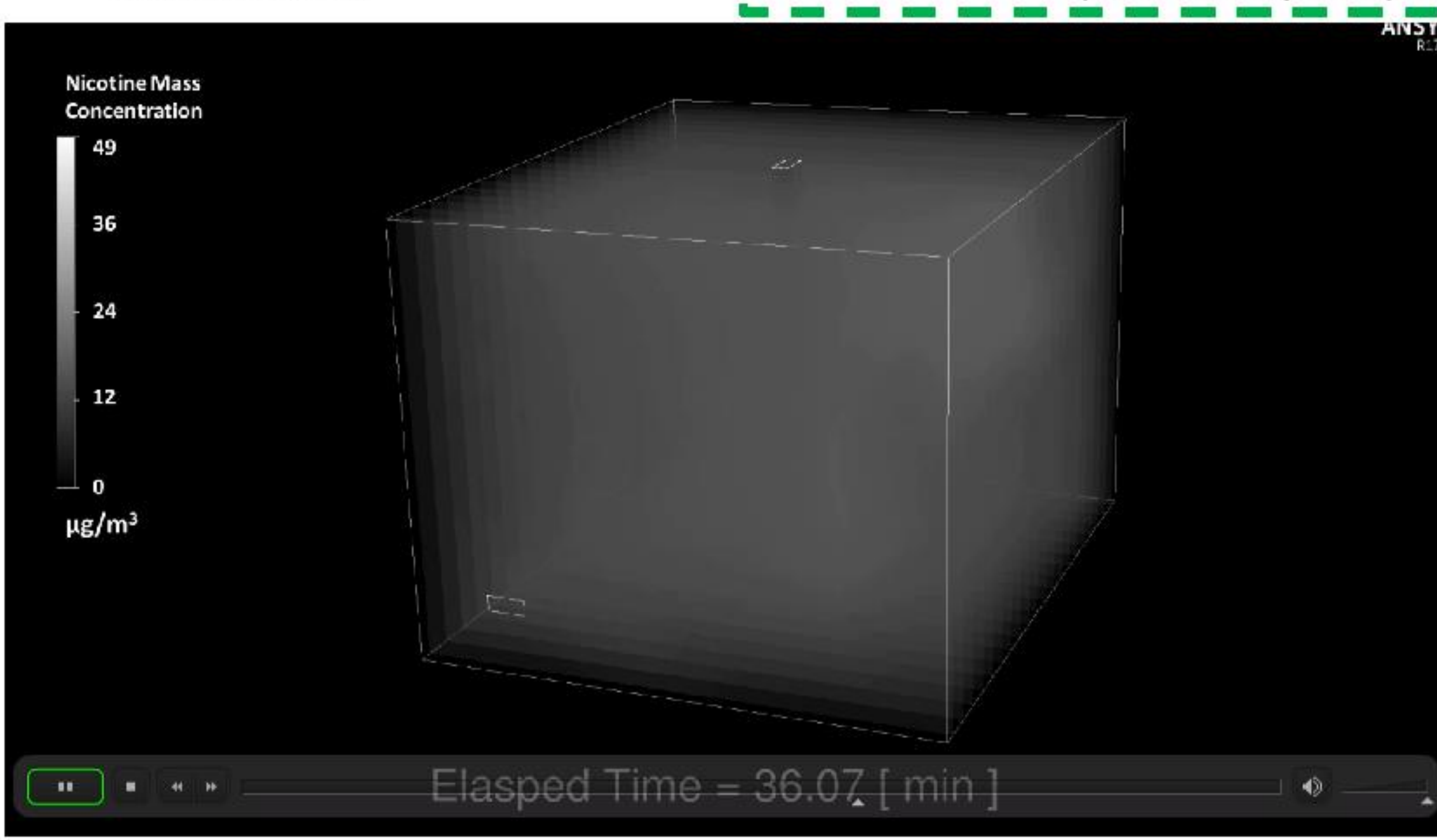
- 2 aerosol doses released in 1 hour
- 15 Puffs in each dose for 3 minutes
- Ventilation rate: 6.83 ACH



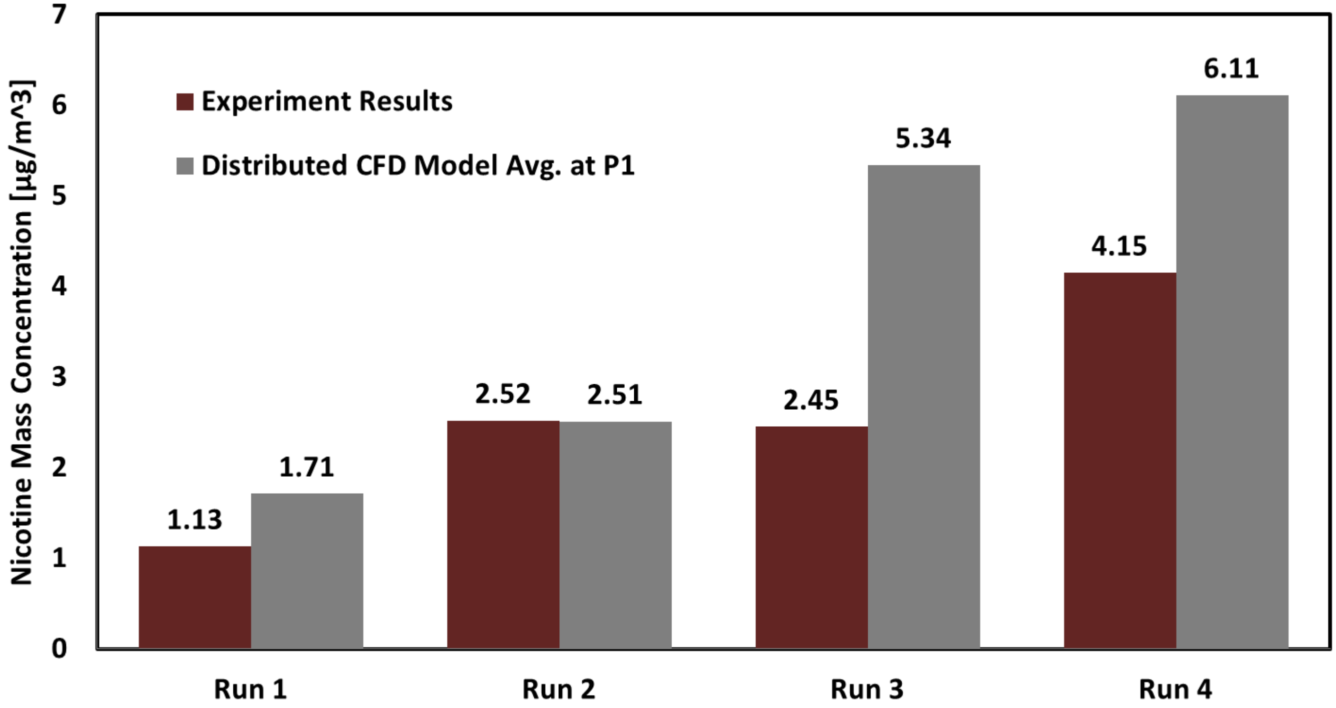
Room Nicotine Concentration Profile

Exhaled E-cigarette
Aerosol Particles





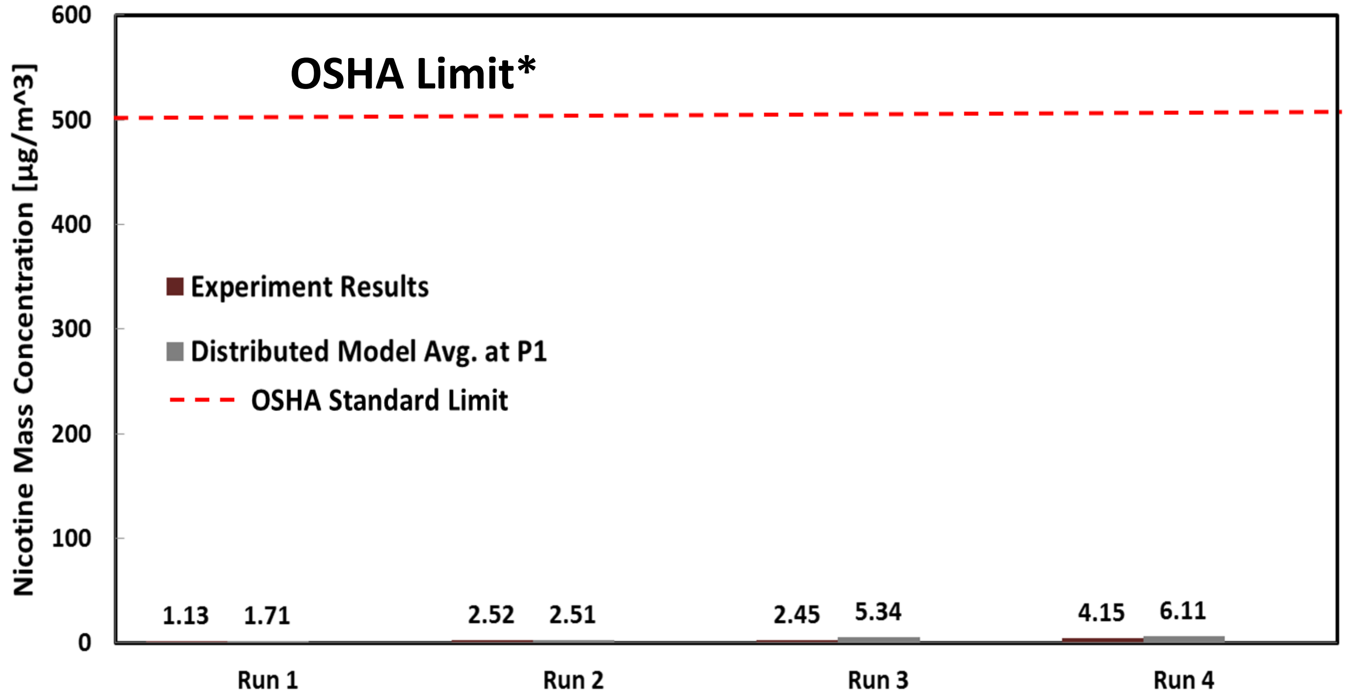
Distributed CFD Model Average vs. Experimental Data



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

ACH= Air Change per Hour *For 8 hour exposure

Distributed CFD Model Average vs. Experimental Data



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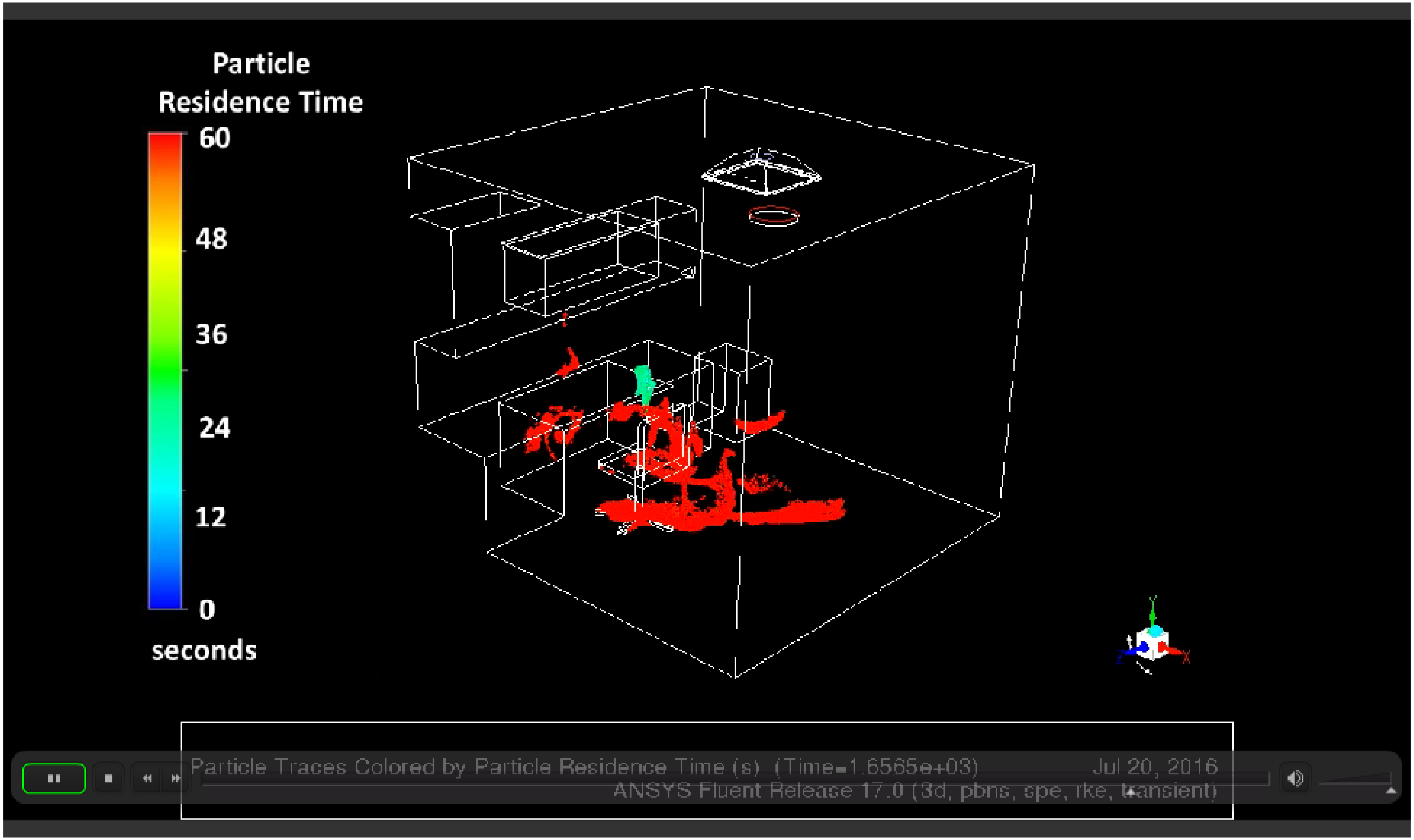
Modeling Example 1: Office Space Aerosol Circulation Profile



- 10 Puffs in 30 minutes
- Ventilation Rate: 0.35 ACH (ASHRAE Standard)

ASHRAE = American Society of Heating, Refrigerating and Air-Conditioning Engineers

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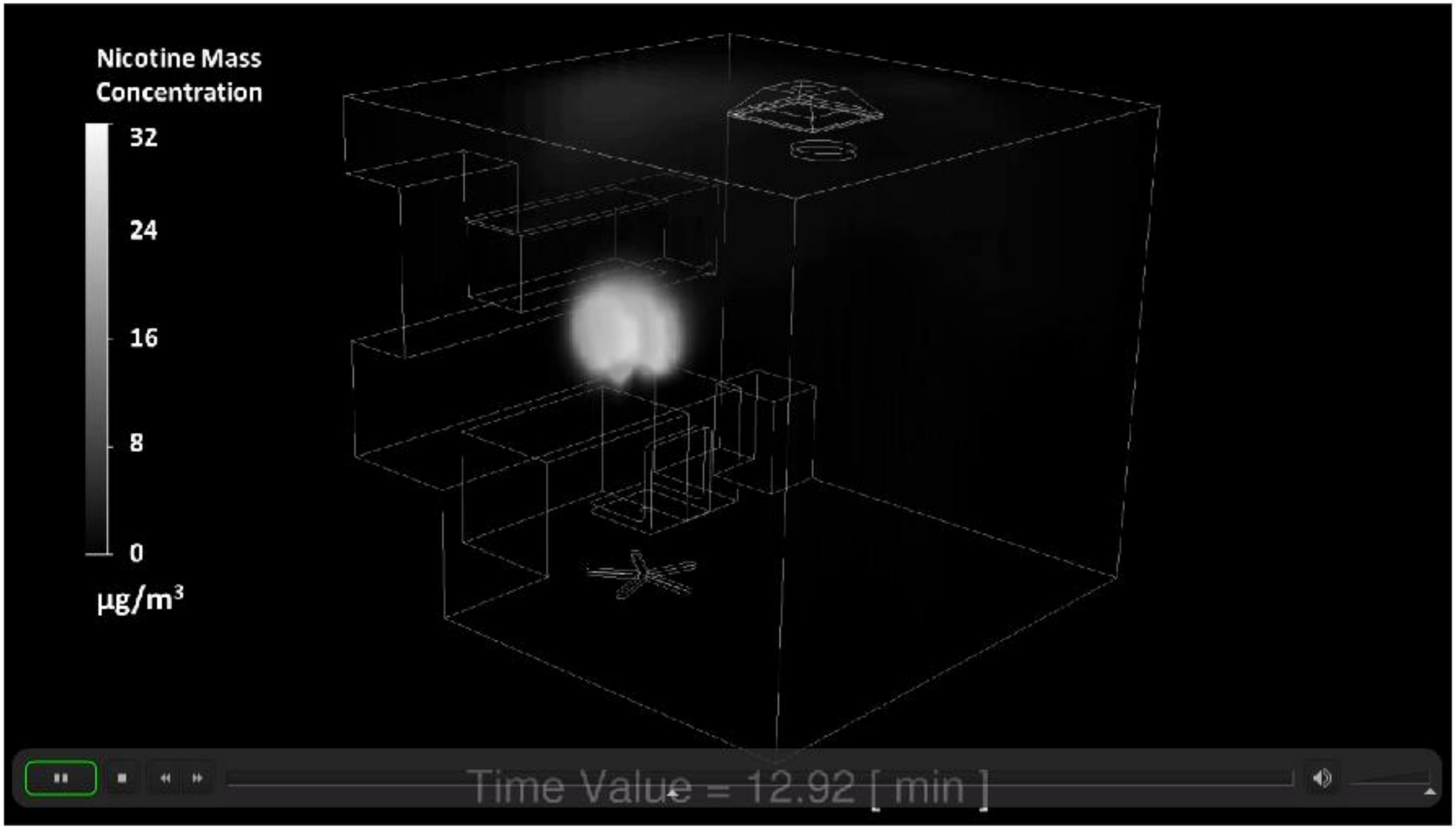
Modeling Example 1: Office Space Nicotine Vapor Concentration Profile



Time-weighted average concentrations over 60 min

Nicotine: 2.30 μg/m³; PG : 76.55 μg/m³; Glycerol : 102.96 μg/m³

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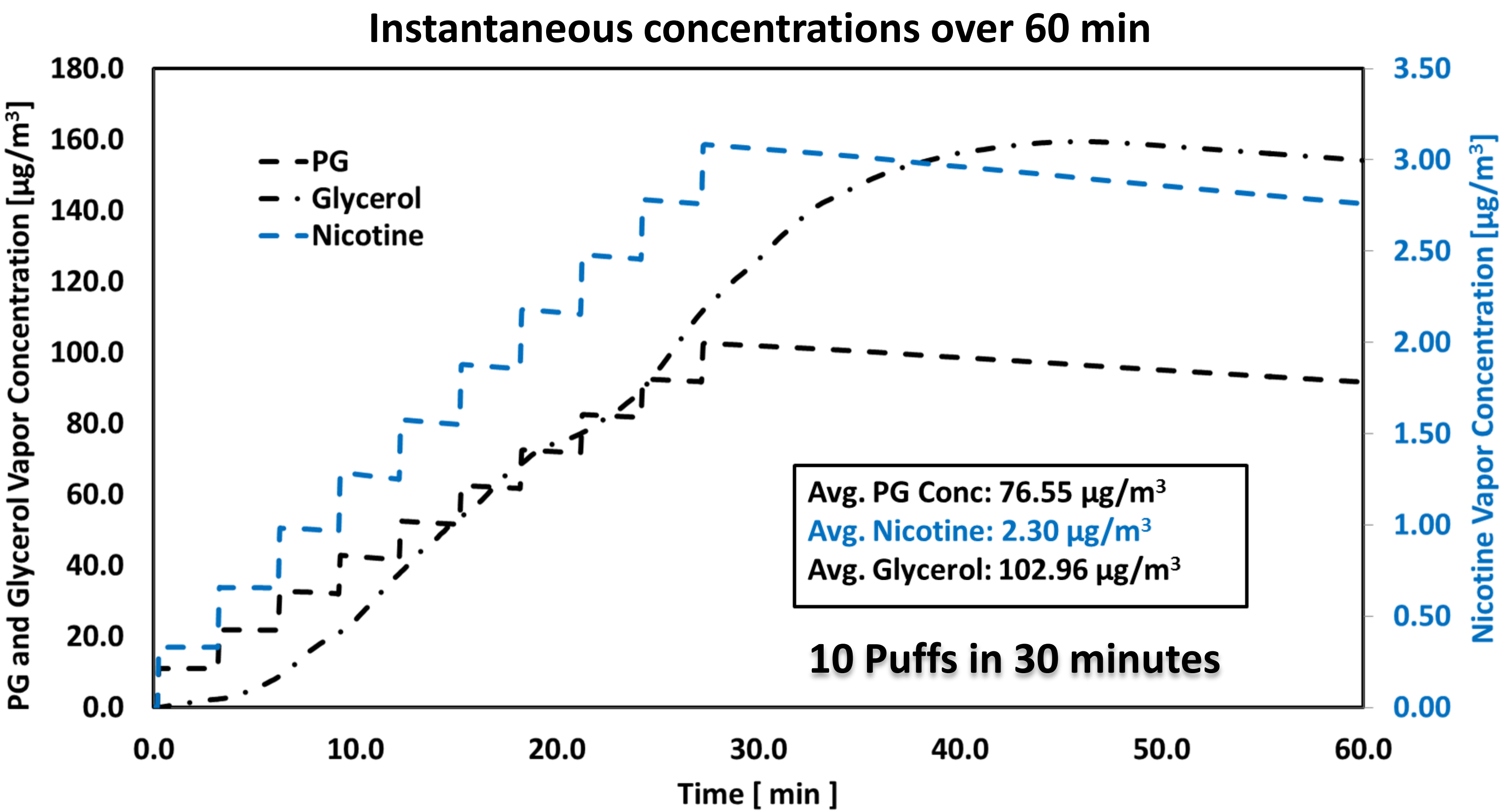
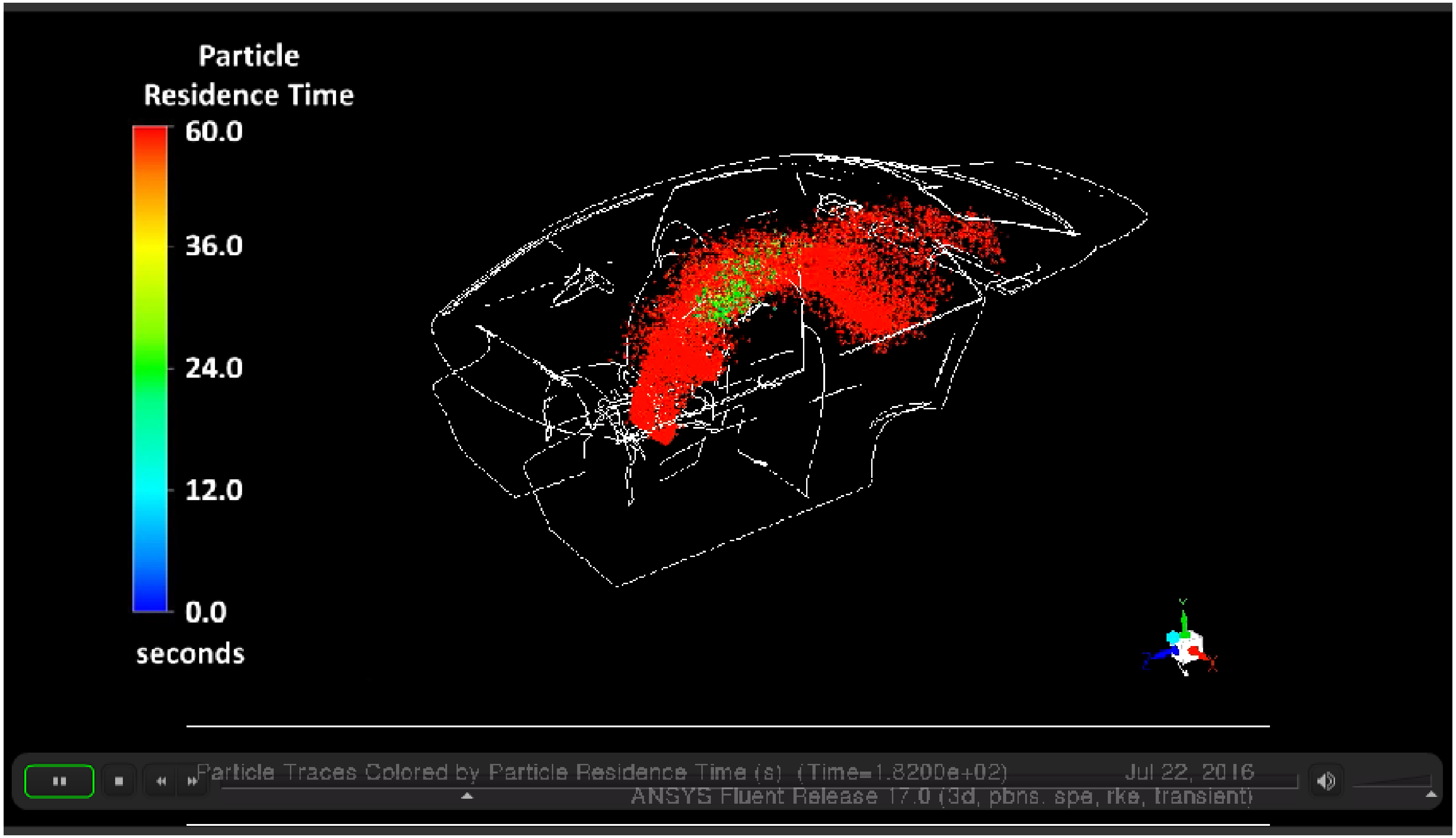
**OSHA Limit for Nicotine (500 μg/m³) and for Glycerol (15,000 μg/m³)*

Modeling Example 1: Office Space Vapor Concentrations



**OSHA Limit for Nicotine (500 µg/m³) and for Glycerol (15,000 µg/m³)*

Modeling Example 2: Car Cabin Aerosol Circulation Profile with Windows Closed



- 10 Puffs in 10 minutes
- Ventilation rate: 3.23 ACH*

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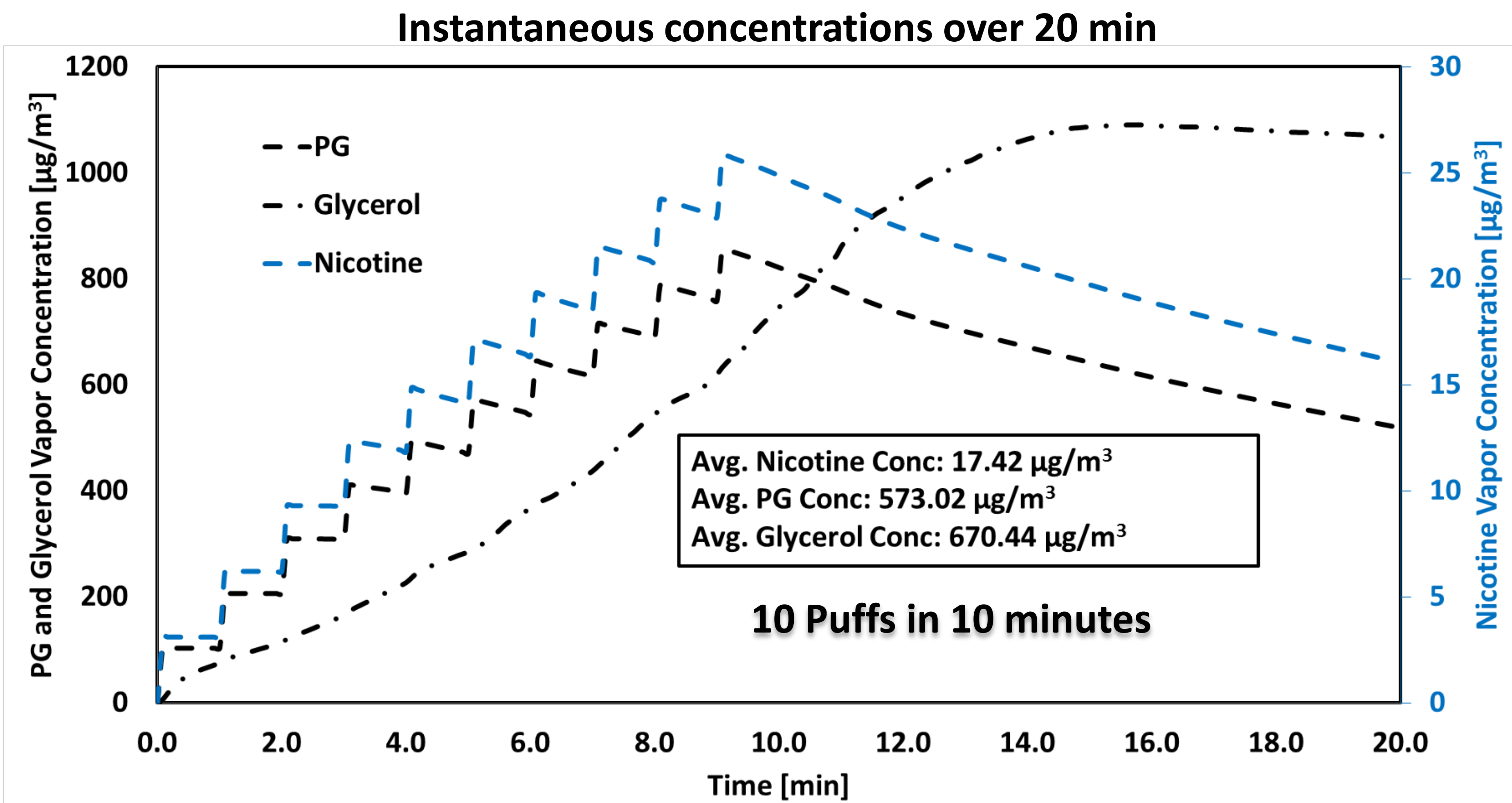
*Wayne et al. (2008) Air change rates of motor vehicles and in-vehicle pollutant concentrations from secondhand smoke.

Modeling Example 2a: Car Cabin Vapor Concentrations with Windows Closed



OSHA Limit for Nicotine (500 µg/m³) and for Glycerol (15,000 µg/m³)

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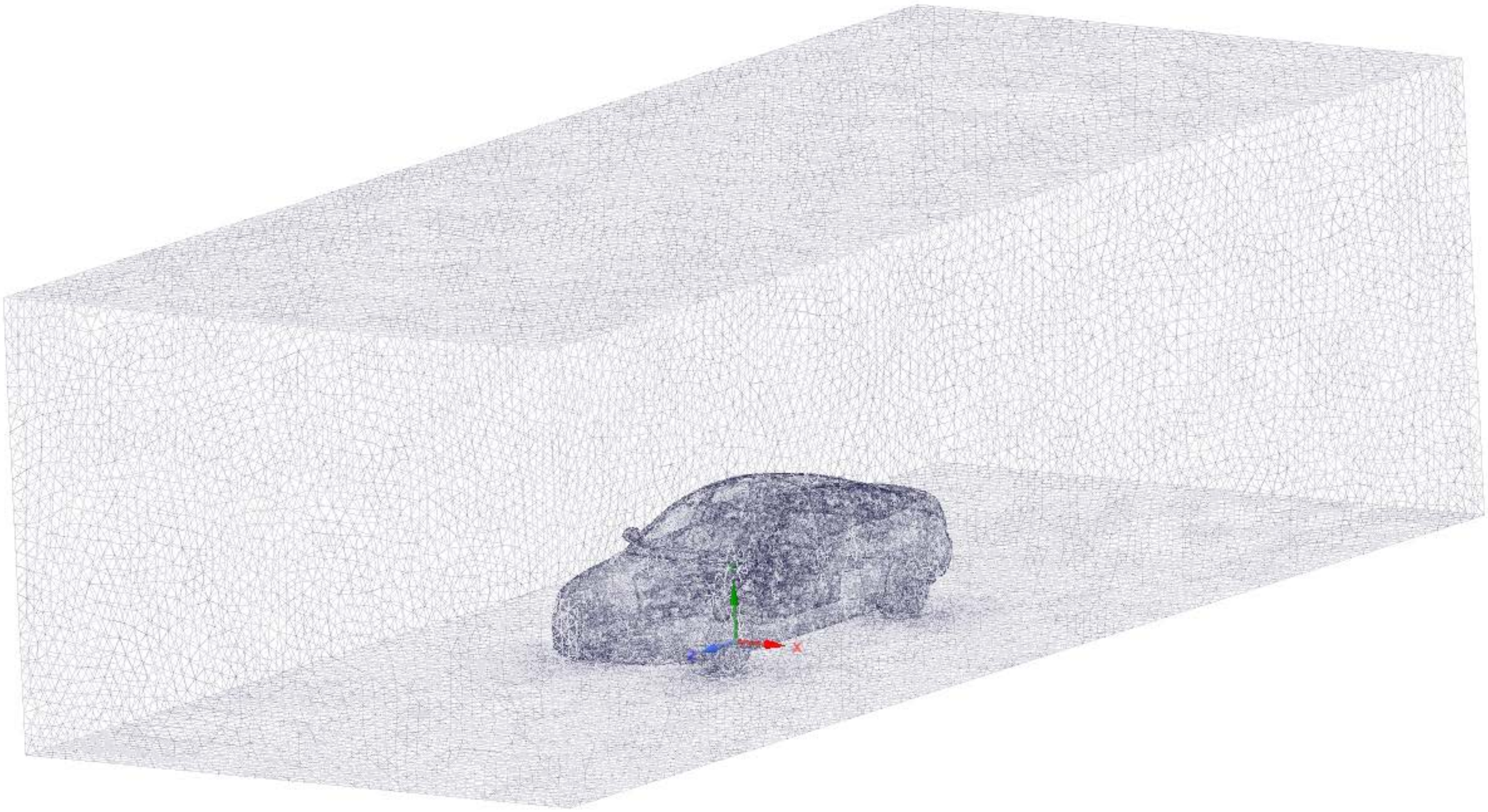
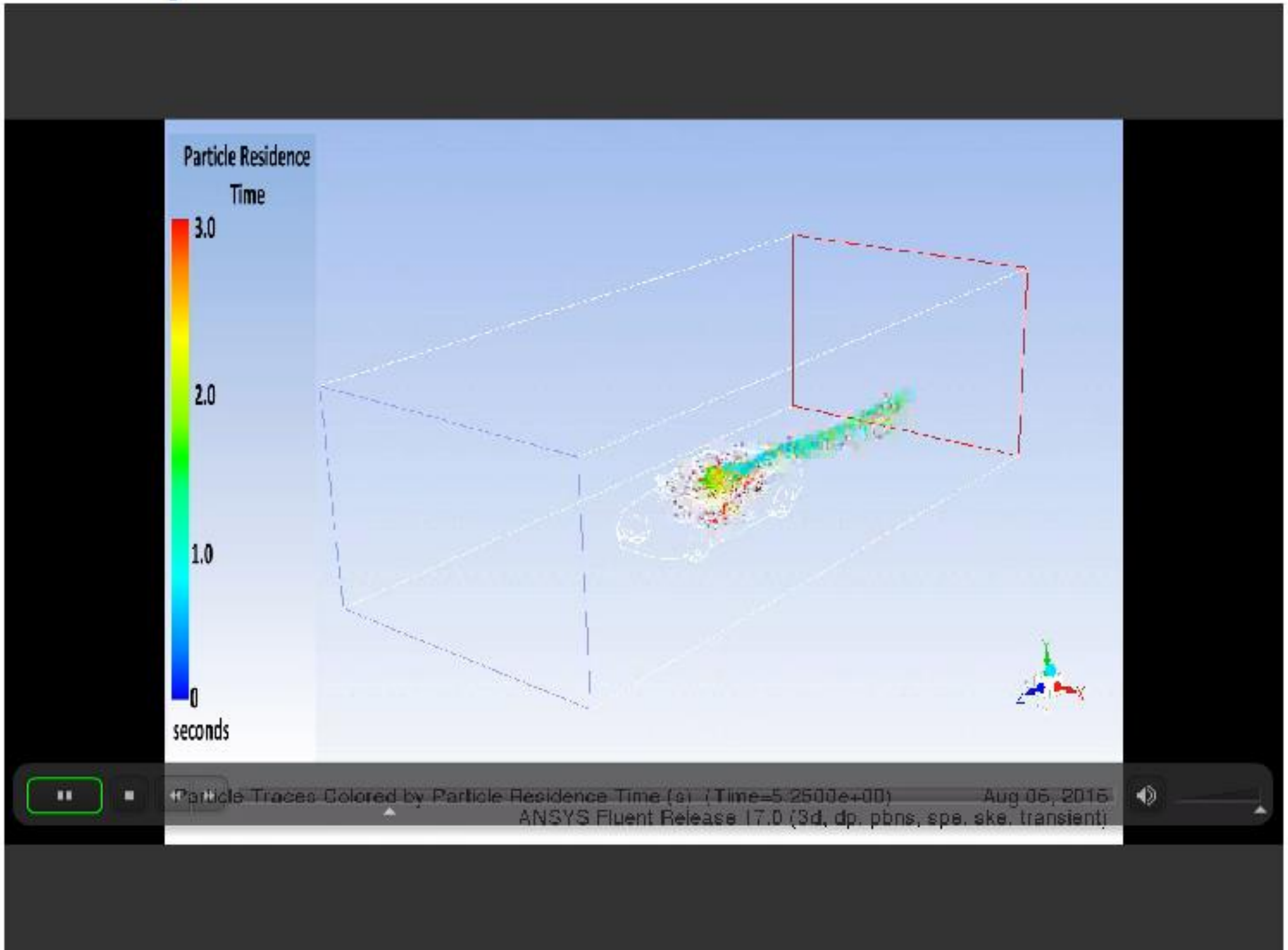
Model Application Example 2b: Geometry/Mesh for Car with open Windows



Modeling Example 2b: Car Cabin Aerosol Circulation Profile with Windows Open



- 10 Puffs in 10 minutes
- Vehicle traveling at 35mph; windows fully opened

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Modeling Example 2b: Car Cabin Vapor Concentrations with Windows Opened

Aerosol Vapor Constituents	Average Concentration (µg/m^3)
Nicotine	0.0021
PG	0.0695
Glycerol	0.0860

***OSHA Limit for Nicotine (500 µg/m^3) and for Glycerol (15,000 µg/m^3)**

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Summary

- We developed computational models to estimate room air concentration of constituents from e-cigarette use
- The model can be used to estimate the secondhand exposure level in a variety of use conditions and indoor settings
- Results from modeling can be used to better inform and strengthen the scientific understanding to evaluate and regulate electronic cigarettes
- We plan to continue sharing our progress with the scientific community

Thank You

Copy of presentation available at ALCS Science website:

http://www.altria.com/ALCS-Science

Addendum: Notations for Equations

ACH	Air Change per Hour	h^{-1}
UDF	User Defined Function	
P_{r_T}	Turbulent Prandtl Number	Dimensionless
Sc_T	Turbulent Schmidt Number	Dimensionless
ν_T	Turbulent Viscosity	Pa s
C_p	Specific Heat Capacity	kJ/kgK
T	Temperature	K
T_p	Particle Temperature	K
$S^{(E)}$	Energy Source Term	
S_i	Mass source term for constituent i	
ρ	Density	kg/m^3
k	Thermal Conductivity	W/mK

$k_{m,i}$	Mass transfer coefficient of constituent i	
v	Velocity	m/s
t	Time	s
$S_i^{(E)}$	Energy source/sink for species i	
$S_i^{(Y)}$	Mass source term for constituent i	kg/m^3s
n_c	Total number of Particles in a computational cell	
d_p	Particle Diameter	m
m_p	Particle Mass	kg
u_p	Particle Velocity	m/s
J_i	Mass Flux of Constituent i	kg/m^2s
H_i	Latent Heat of Species i	kJ/mol
h_i	Enthalpy of Species i	
D_i	Molecular Diffusivity of i^{th} vapor constituent	

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Addendum: Notations for Equations (Cont.)

A_i, B_i, C_i, D_i, E_i	Antoine Equation Constants for each species i	
$T_{c,i}$	Critical Temperature of constituent i	K
C_i	Mass concentration of vapor constituent i	kg/m^3
$C_{i,s}$	Vapor species concentration on particle surface	
n_i	Constant	
V_c	Computational Cell Volume	m^3
F^D	Drag Force	N
F^L	Lift Force	N
F^{BM}	Brownian Motion Force	N
F^G	Gravity Force	N
R	Universal Gas Constant	$m^3Pa/molK$
M	Molecular Mass	kg/kmol
M_i	Molecular Mass of constituent i	kg/kmol
γ_i	Activity Coefficient of constituent i	Dimensionless
x_i	Mole Fraction of constituent i	
y_i	Mass Fraction of constituent i	
$Y_{i,s}$	Mass fraction of vapor constituent i at the particle surface	
P_{sat}	Saturated Vapor Pressure	kg/ms^2
Sh	Sherwood Number	Dimensionless
Re	Reynolds Number	Dimensionless

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