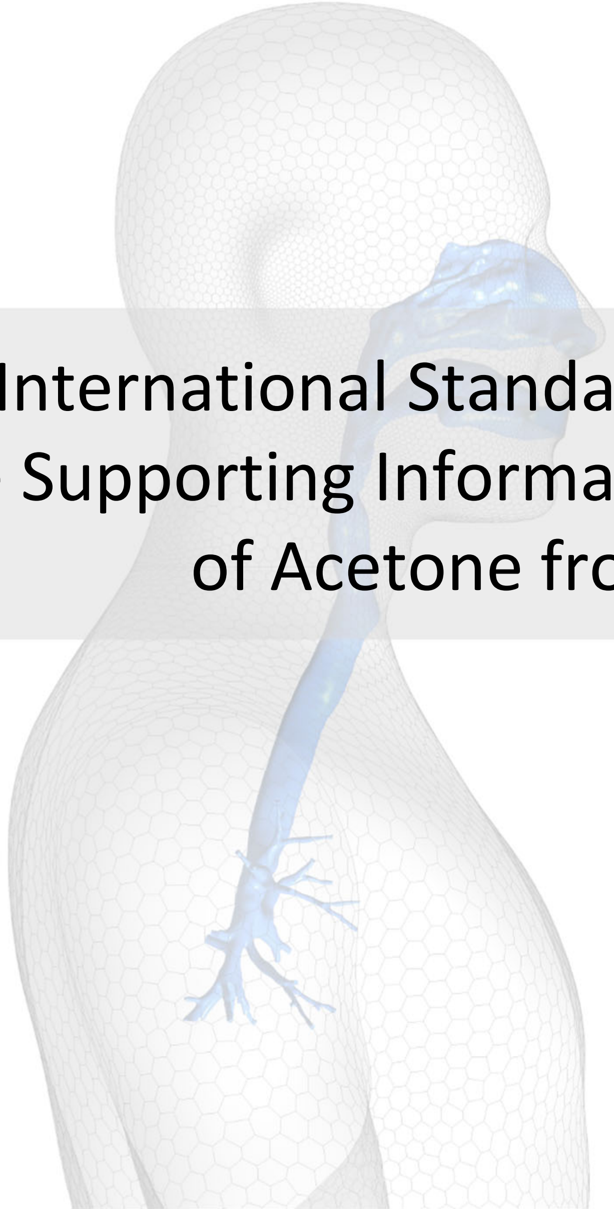

International Standardization of Testing Perceived Air Quality and the Supporting Information from *in silico* model for Transport Efficiency of Acetone from Indoor to Olfactory Epithelium Cells

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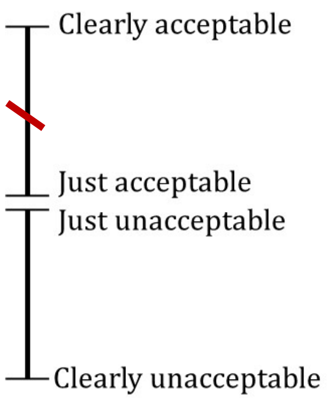
Smell/ Odour in Indoor Environment

- Perceived Air Quality / Bio-effluent
- Convener ISO TC146/SC6/WG25
  – ISO FDIS 16000-44 “Test method for measuring perceived indoor air quality for use in testing the performance of gas phase air cleaners”

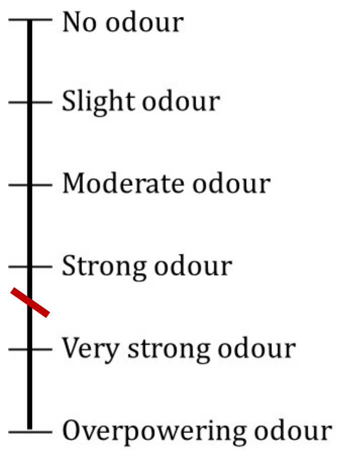

How many sniffs for subjective evaluation?

ISO FDIS 16000-44

- ISO TC146 (Air Quality) /SC6 (Indoor Air) /WG25 (Air Cleaning Technology)
  - Test method for measuring perceived indoor air quality for use in testing the performance of gas phase air cleaners
- Principle for measuring perceived air quality
  - The perceived air quality is determined using subjective evaluations of acceptability and odour intensity. The air assessed by a panel is presented via sniffing device (a funnel).



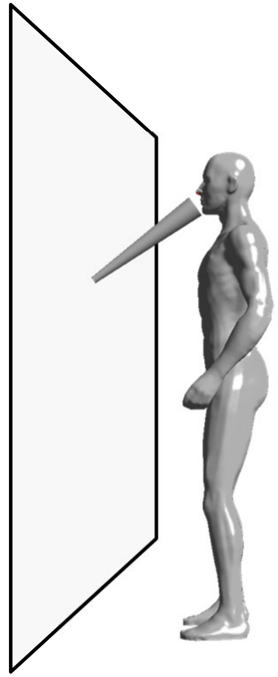
Acceptability scale

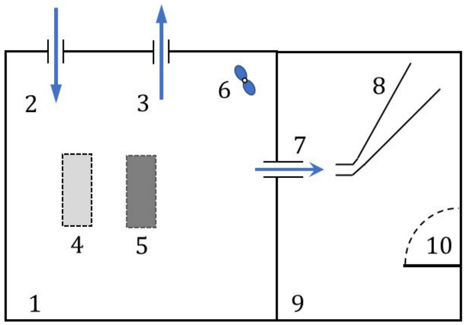


Odour intensity with category scale

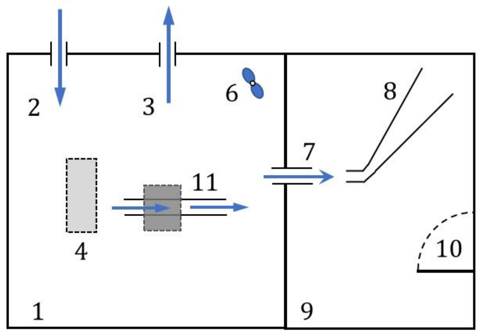
Test Conditions

- The panel member shall enter the front space and assess quality of air presented via sniffing device immediately upon arriving at the measuring point.
- The measurement shall be made after taking one sniff of the air.
- Only one measurement shall be made at a time, either acceptability or perceived odour intensity

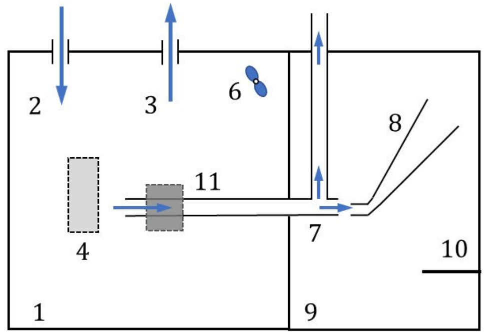




A test room for
a standalone air cleaner



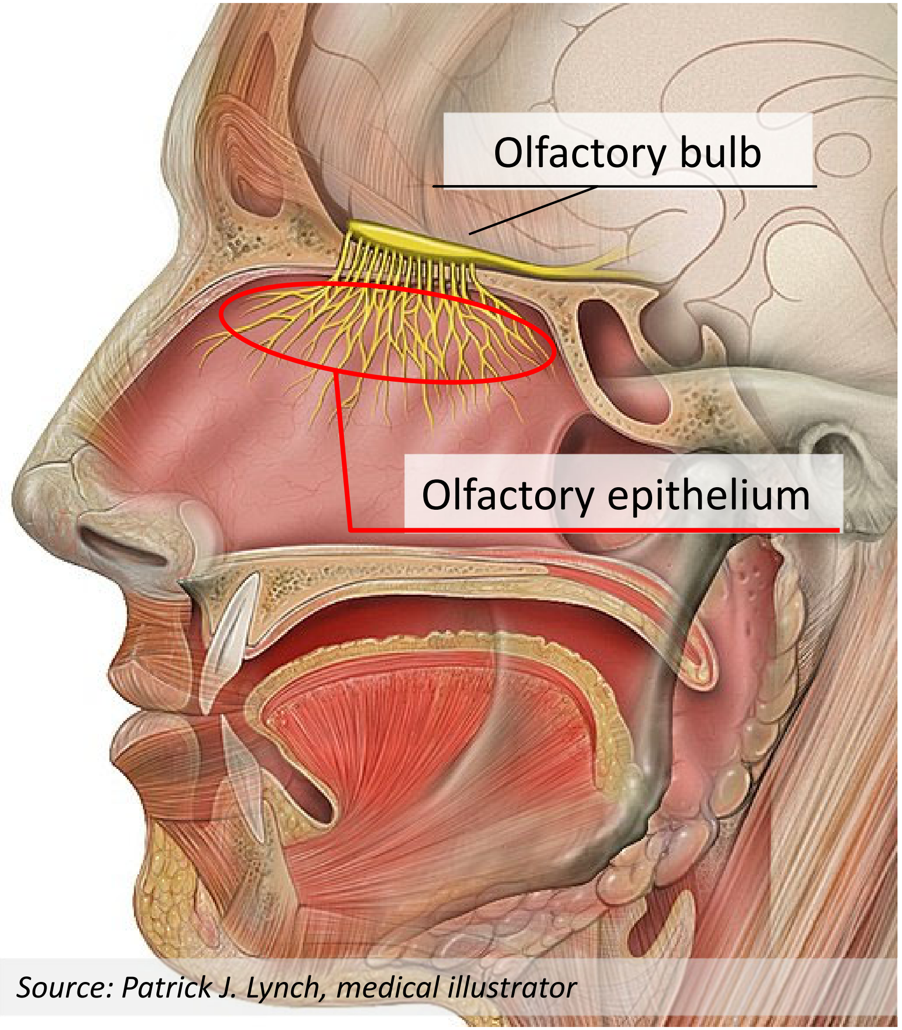
A test room for
a in-duct air cleaner



A test room for
a in-duct air cleaner (single-pass condition)

1	test chamber	7	tube or duct
2	clean and temperature/humidity conditioned air supply inlet	8	sniffing device
3	exhaust outlet	9	front/anterior space in which human panel enter
4	emission source	10	Doors where panel enters
5	An air cleaner	11	in duct air cleaner
6	mixing fan		

Perception of Odour/ Smell



Source: Patrick J. Lynch, medical illustrator

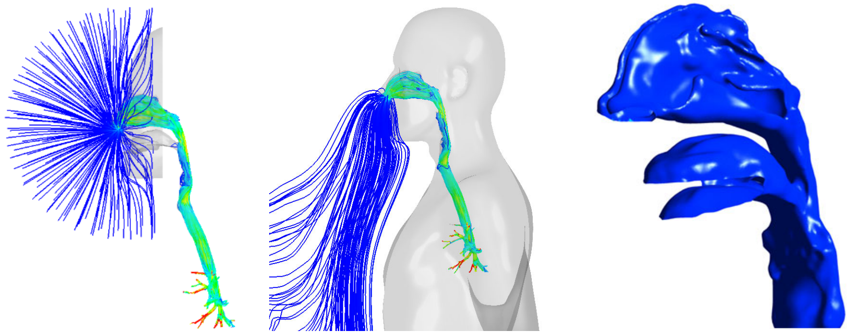
Sensory experiment

- Direct volunteer participant(s) evaluation/ high sensitivity
- Ethical constraints

Odor Intensity level	
extremely strong	6
very strong	5
strong	4
distinct	3
weak	2
very weak	1
no odor	0

CFD based *in silico* Approach

- Analysis for physico-chemical mechanism
- Analysis for Hygrothermal-chemical transfer mechanism



Modeling the Wall Surface Decomposition/Deposition Flux of Scalar

- Heterogeneous reaction between Scalar and wall surface
- The surface deposition of the local scalar concentration close to the surface (molecular theory)

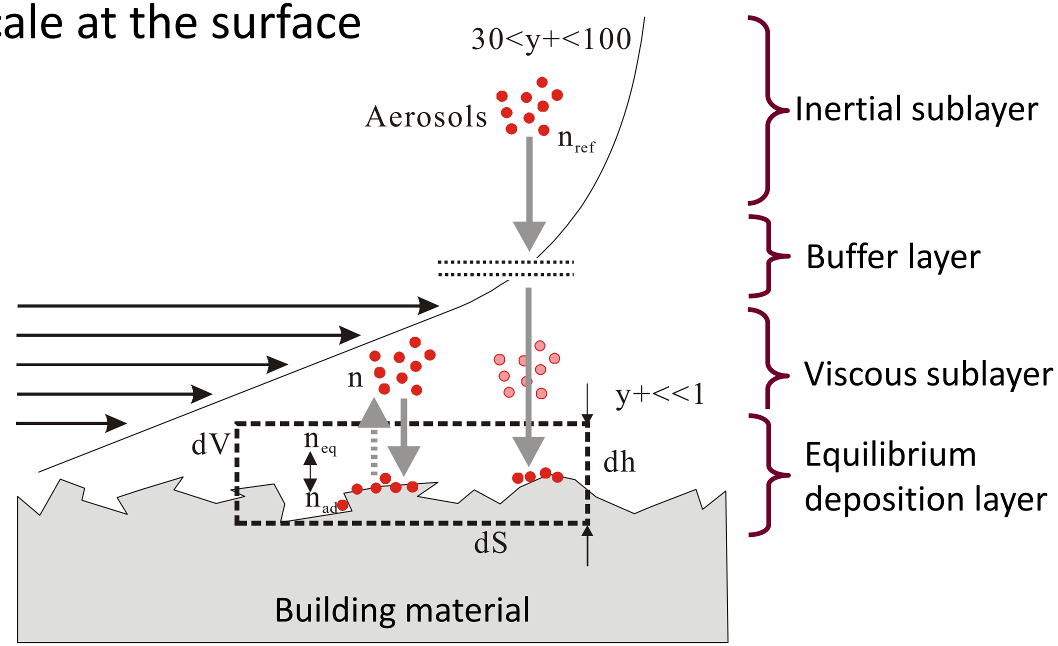
$$Js = -\gamma \frac{\langle v \rangle}{4} C_o \Big|_{y=\frac{2}{3}\lambda}$$

γ [-] : mass accommodation coefficient/Reaction probability

- The flux model to enable an increased length scale at the surface

$$Js = -\frac{\gamma \cdot \frac{\langle v \rangle}{4}}{1 + \gamma \cdot \frac{\langle v \rangle}{4} \cdot \frac{\Delta y_1}{D_o}} \cdot C_o \Big|_{y=\Delta y_1}$$

(damping due to molecular diffusion in viscous sub layers)

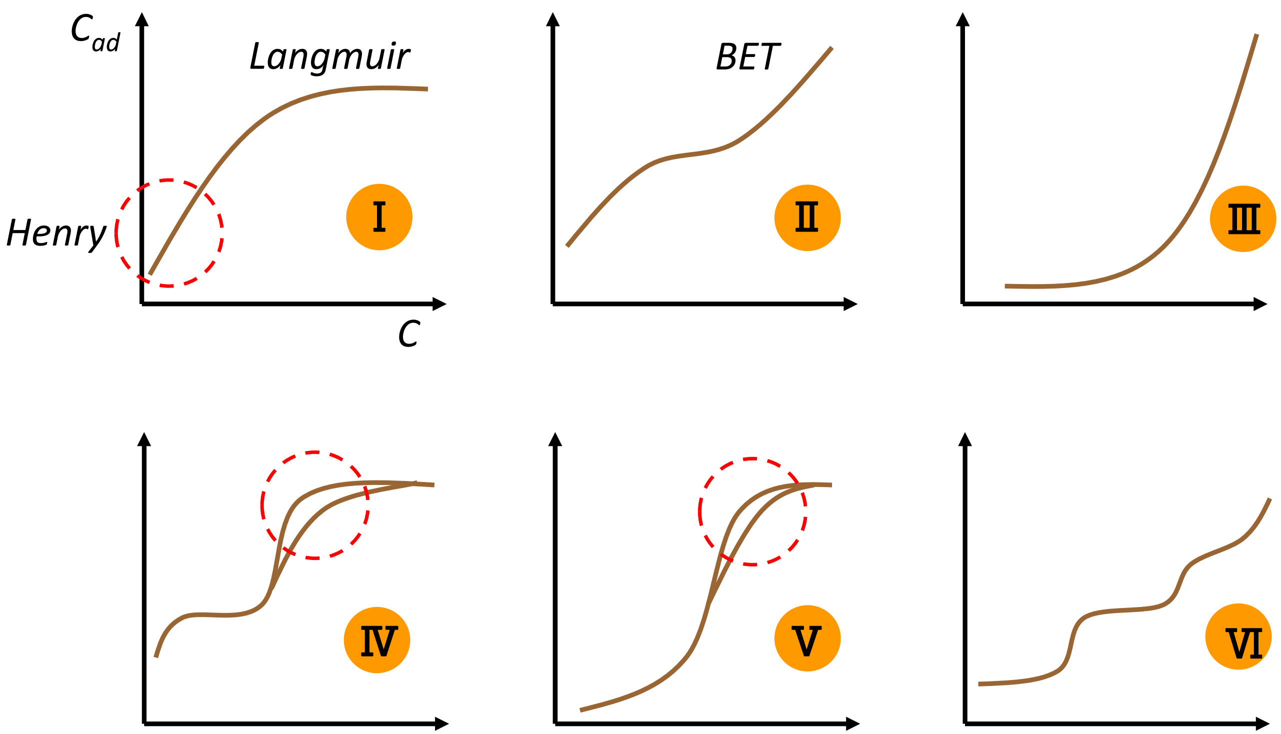


$<v>$ [m/s] : Boltzmann velocity for targe scalar

λ [m] : mean molecular free path (order of the 10^{-8}

Δy_1 : distance to the first computational cell (< y^+=1)

Variety of Adsorption Isotherm



Classification of Adsorption Isotherm
IUPAC (*International Union of Pure and Applied Chemistry*)

Henry type

$$C_{ad} = k_h \cdot C_{eq} = k_h \cdot C$$

Langmuir type

$$C_{ad} = \frac{C_{ad\,0}\, k_l C}{1 + k_l C}$$

BET type

$$C_{ad} = \frac{C_{ad\,0} k_{BET} C_r}{(1 - C_r)(1 - C_r + k_{BET} C_r)}$$

Freundlich type

$$C_{ad} = k_f C^{1/n}$$

Physiologically Based Pharmaco-Kinetic (PBPK) model

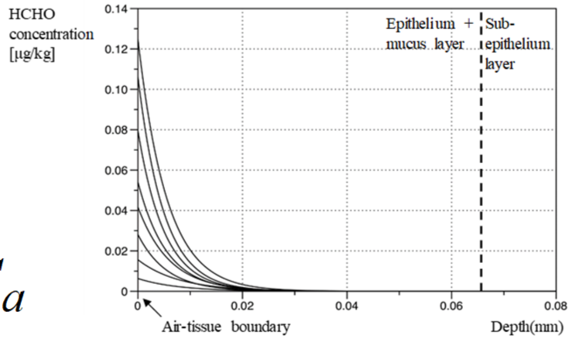
Reaction Diffusion System

Lumen-Tissue Boundary (Flux Conservation)

$$D_a \frac{\partial C_a}{\partial n} = D_t \frac{\partial C_t}{\partial n}$$

partitioning

$$C_t = P_{t:air} C_a$$



HCHO concentration distribution in tissue(0~3sec)

Mucosa + Epithelial

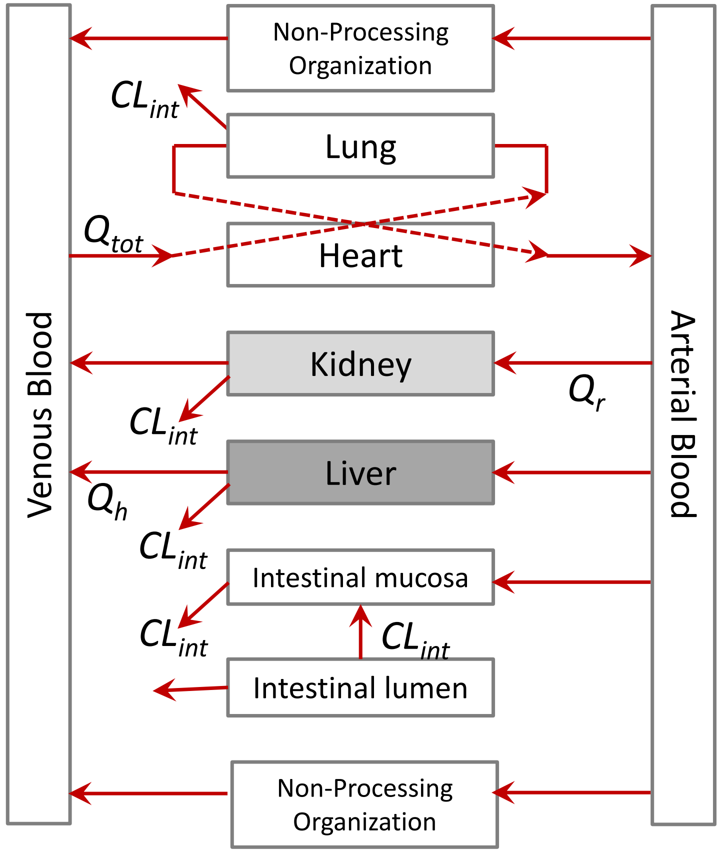
$$\frac{\partial C_t}{\partial t} = -\underbrace{\frac{(V_{\max 1C})C_t}{K_{m1} + C_t}}_{\text{Michaelis–Menten kinetics}} - K_f C_t - K_b C_t + \underbrace{D_t \nabla^2 C_t}_{\text{Diffusion Term}}$$

$$C_b = P_{b:t} C_t$$

Sub-mucosal

$$\frac{\partial C_b}{\partial t} = -K_f C_b - K_b C_b - (Q_b / V_b) C_b + D_b \nabla^2 C_b$$

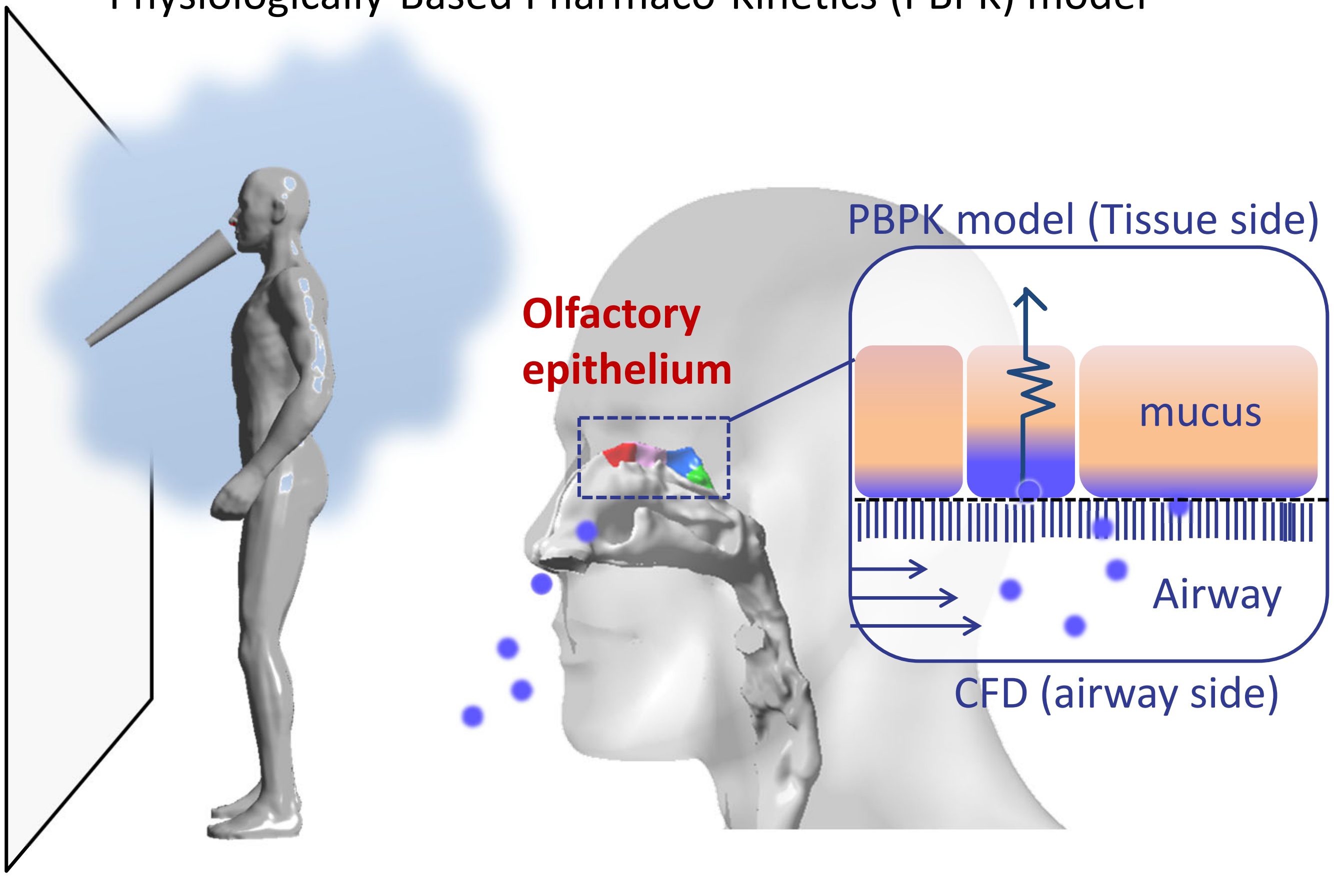
PBPK for Local Tissue/Sites



PBPK for Whole-Body

In Silico Human Model for ISO FDIS 16000-44

- Integrated analysis of flow, heat, moisture, odorous (chemical) substance
- Physiologically-Based Pharmaco-Kinetics (PBPK) model



Reaction-Diffusion equation in 3 layers

Subepithelial tissue

$$\frac{\partial C_b(x,t)}{\partial t} = \frac{\partial^2 C_b(x,t)}{\partial x^2} - \frac{Q_b}{V_b} C_b(x,t)$$

C_{sub}

Epithelial tissue

$$\frac{\partial C_t(x,t)}{\partial t} = D_t \frac{\partial^2 C_t(x,t)}{\partial x^2}$$

C_{epi}

Mucus

$$\frac{\partial C_m(x,t)}{\partial t} = D_m \frac{\partial^2 C_m(x,t)}{\partial x^2}$$

$C_{m,0}$

Airway lumen (CFD)

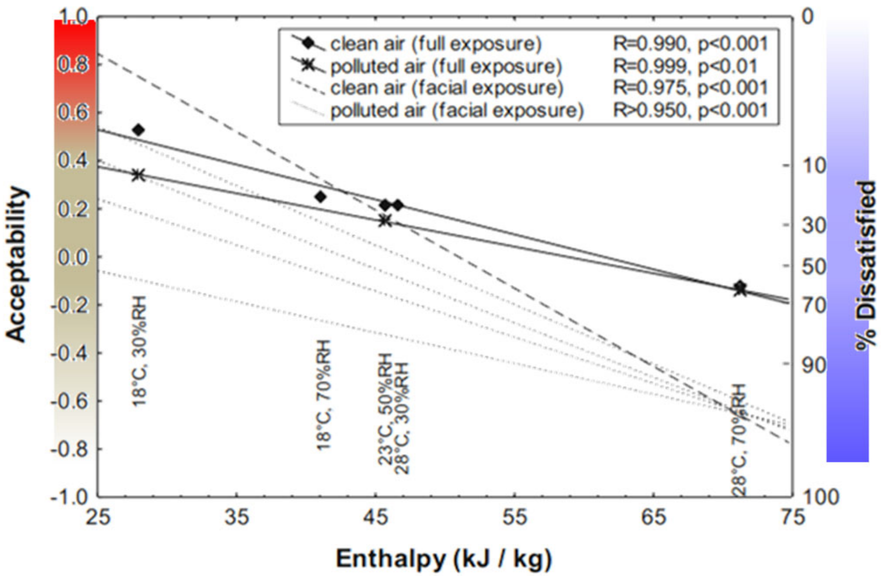
$$\frac{\partial \overline{C_a}}{\partial t} + \frac{\partial \overline{U_i C_a}}{\partial x_i} = \frac{\partial}{\partial x_i}\left\{\left(D_a + \frac{\nu_t}{\sigma_t}\right)\frac{\partial \overline{C_a}}{\partial x_i}\right\}$$

Adsorption equilibrium

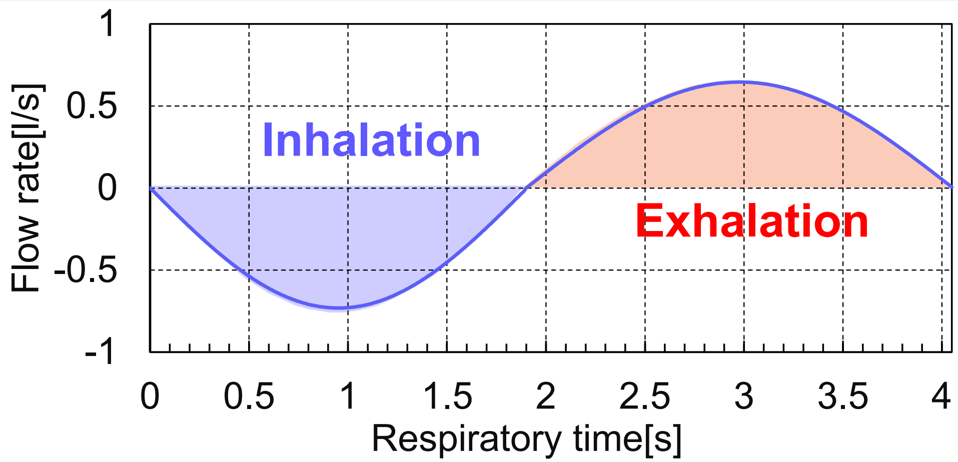
$$\begin{cases} C_{sub} = P_{epi,sub} C_{t,n} \\ C_{epi} = P_{m,epi} C_{m,n} \\ C_{m,0} = P_{m:air} C_{air,0} \end{cases}$$

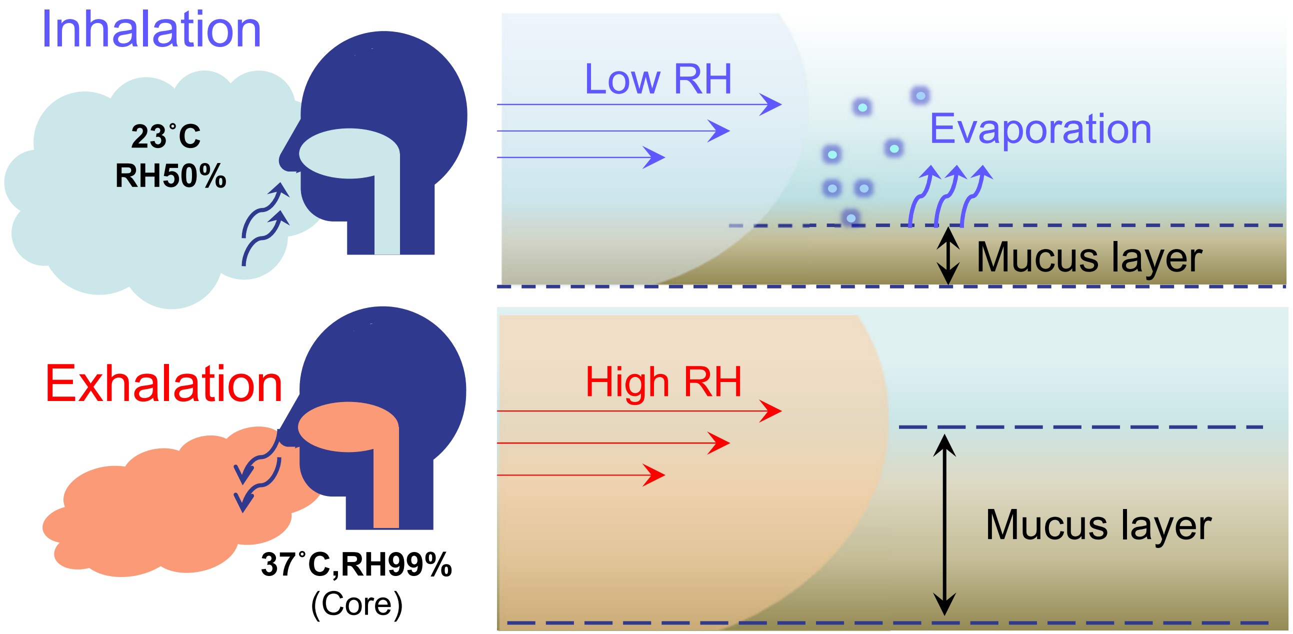
Thermo-Regulation / Heat and Mass Transfer

- Enthalpy of indoor air will affect odour perception
- As the enthalpy of indoor air increases, acceptability decreases and the % dissatisfied increases.



(Fang L, Clausen G, Fanger PO, *Indoor Air*, 1998)





Thermo-Regulation model for Skin Surface and Core Temperature Control

- Heat Balance of Human Body

$$
\left.\begin{aligned}
M &= Q_{sk} + Q_{res} + S \\
&= (Q_{cv} + Q_r + E_{sk}) + (C_{res} + E_{res}) + S_{cr} + S_{sk}
\end{aligned}\right\}
$$

$$
\begin{aligned}
M &= 0.0014M(34-\theta_a) - 0.000017M(5867-p_a) \\
&\quad - 0.00305(5733-6.99M-p_a) + 0.42(M-58.2) + f_{cl}\alpha_c(\theta_{cl}-\theta_a) \\
&\quad + \varepsilon\cdot\sigma\cdot f_{cl}\frac{A_r}{A_D}\left\{(\theta_{cl}+273)^4 - (MRT+273)^4\right\}
\end{aligned}
$$

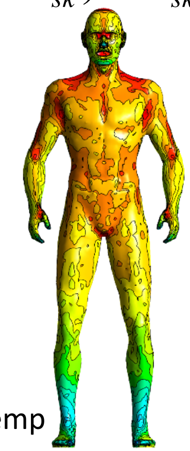
Comfort equation (by Fanger)

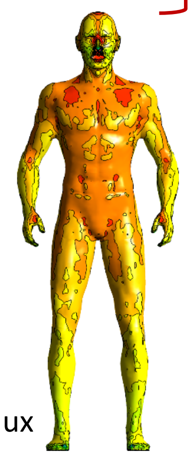
- Heat storage in Core and Skin (Gagge's two node concept)

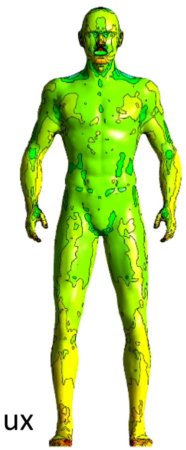
$$
\left.\begin{aligned}
S_{cr} &= M - C_{res} - E_{res} - K(t_{cr} - t_{sk}) - c_{p,bl}m_{bl}(t_{cr} - t_{sk}) \\
&= M - C_{res} - E_{res} - (K + c_{p,bl}m_{bl})(t_{cr} - t_{sk})
\end{aligned}\right\}
\quad S_{cr} = \frac{(1-\alpha_{sk})m\cdot c_{p,b}}{A_D}\frac{dt_{cr}}{d\theta}
$$

$$
\left.\begin{aligned}
S_{sk} &= K(t_{cr} - t_{sk}) - c_{p,bl}m_{bl}(t_{cr} - t_{sk}) - E_{sk} - (Q_{cv} + Q_r) \\
&= (K + c_{p,bl}m_{bl})(t_{cr} - t_{sk}) - E_{sk} - Q_{cv} - Q_r
\end{aligned}\right\}
\quad S_{sk} = \frac{\alpha_{sk}\cdot m\cdot c_{p,b}}{A_D}\frac{dt_{sk}}{d\theta}
$$

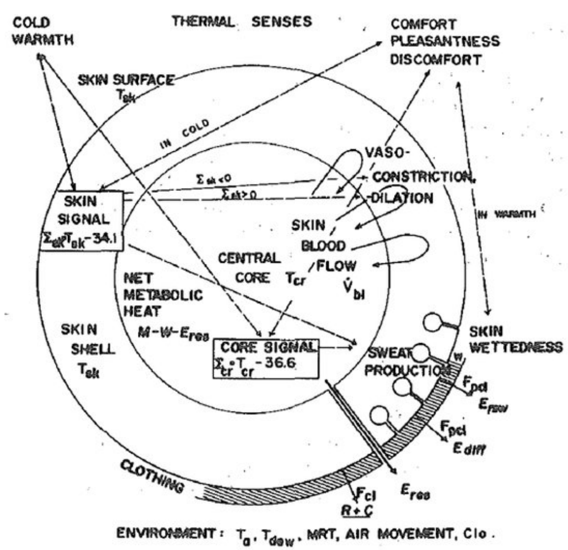

Core temp


Skin surface temp


Sensible heat flux


Latent heat flux

Gagge (1986)



Hygrothermal Transfer Modeling in Respiratory Tract

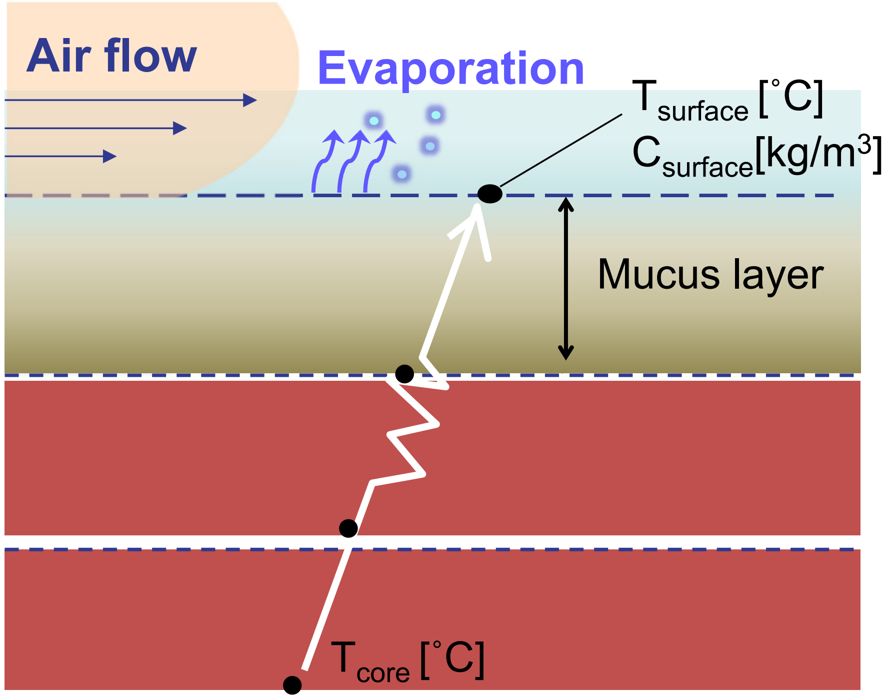
- Total heat balance equation of airway wall

$$\underbrace{k_m \frac{\partial T}{\partial x}}_{\textit{conduction}} = \underbrace{(k_{air} + k_{air,t}) \frac{\partial T}{\partial x}}_{\textit{sensible heat}} + \underbrace{L(D_{air} + D_{air,t}) \frac{\partial C}{\partial x}}_{\textit{latent heat}}$$

- Water vapor concentration on mucus surface

$$C_{surface} = \rho_{air}\left(\frac{0.622e}{p-0.378e}\right) \ [\mathrm{kg/m^3}]$$

$$e = 0.61078\exp\left(\frac{7258.2T_{surface}}{T_{surface} + 237.3}\right) \ [\mathrm{kPa}]$$

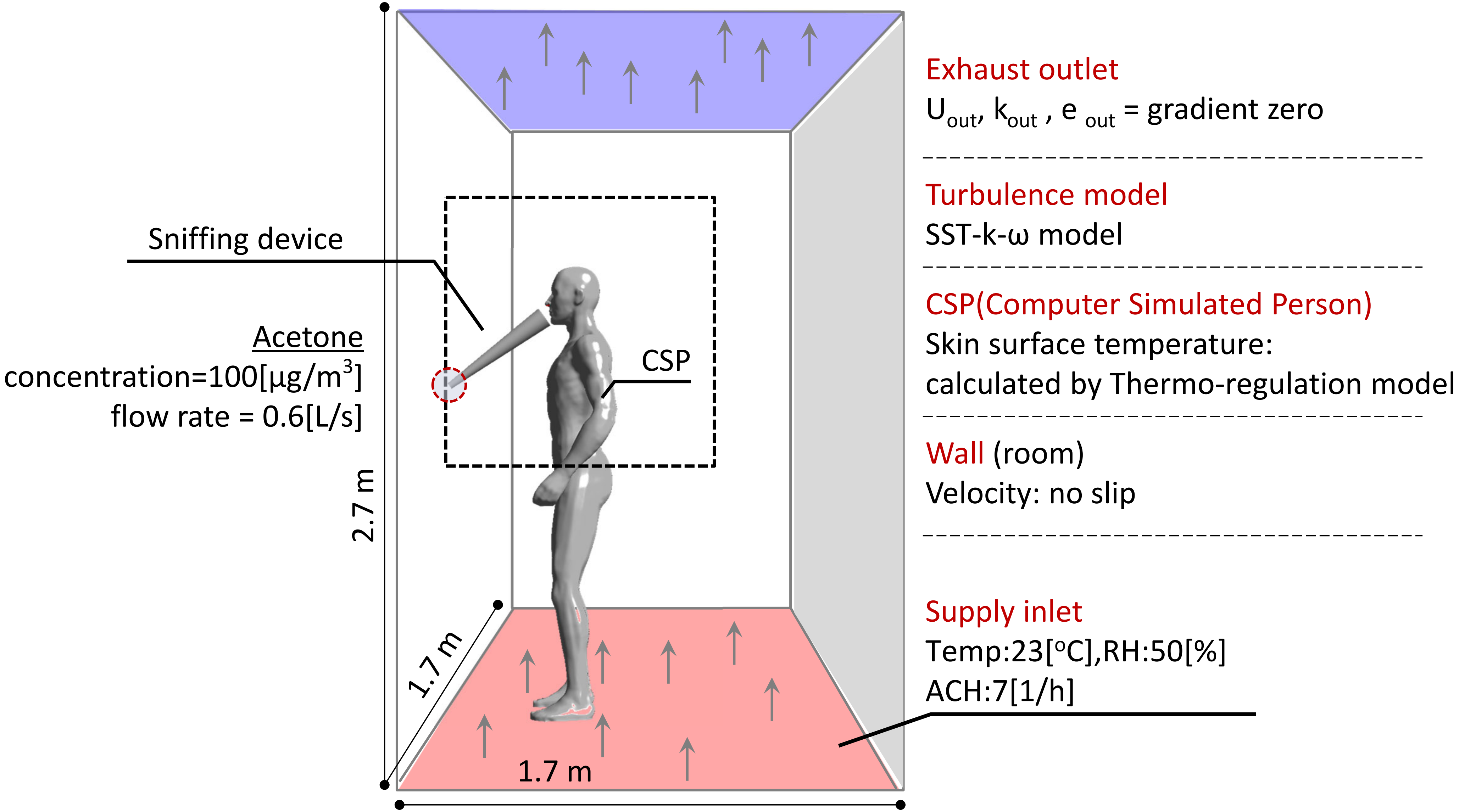


$$S_{cr} = \frac{(1-\alpha_{sk})m \cdot c_{p,b}}{A_D} \frac{dt_{cr}}{d\theta}$$

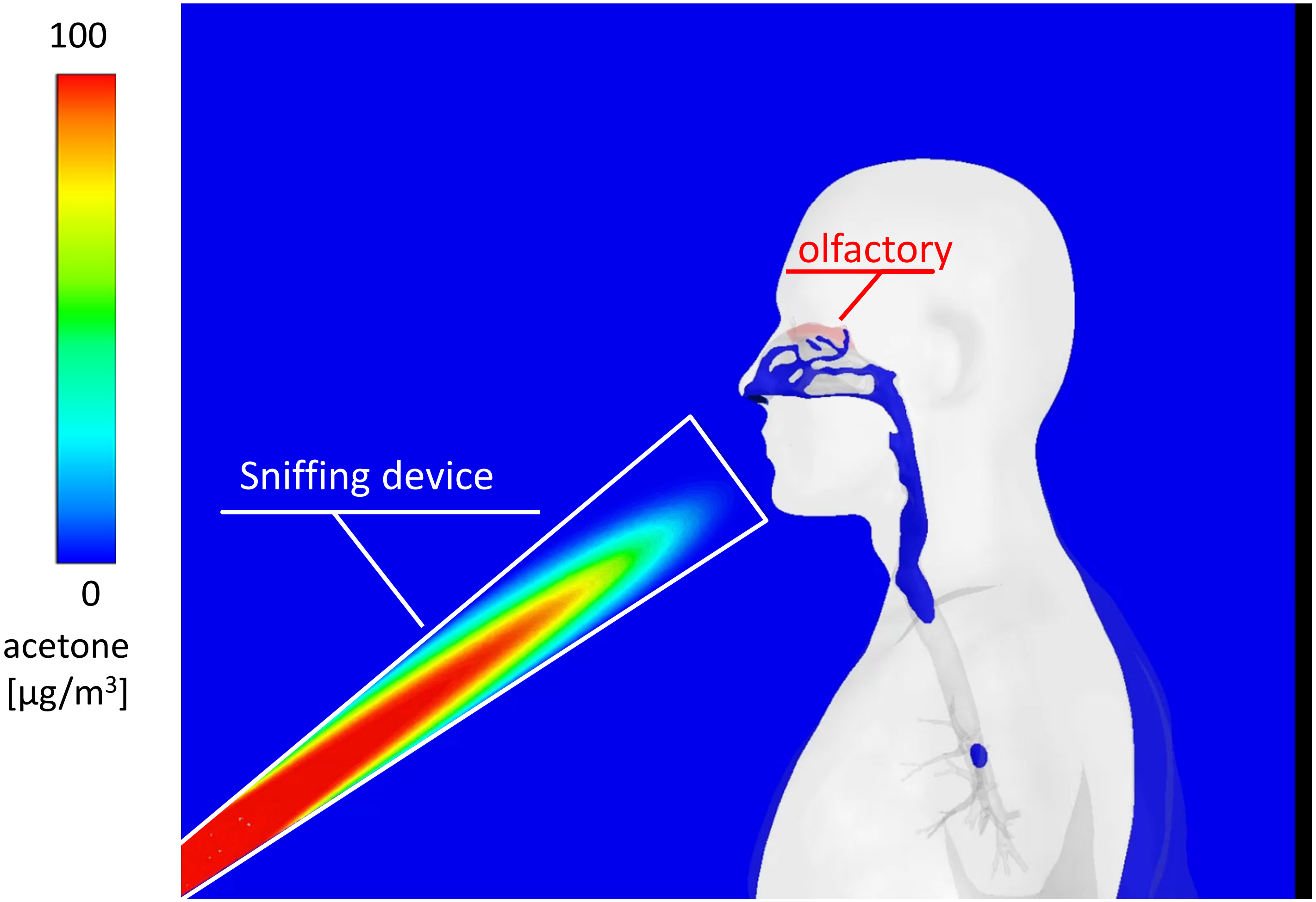
$$S_{sk} = \frac{\alpha_{sk} \cdot m \cdot c_{p,b}}{A_D} \frac{dt_{sk}}{d\theta}$$

CSP with Thermo-regulation (Gagge's two node concept)

Cases Analyzed

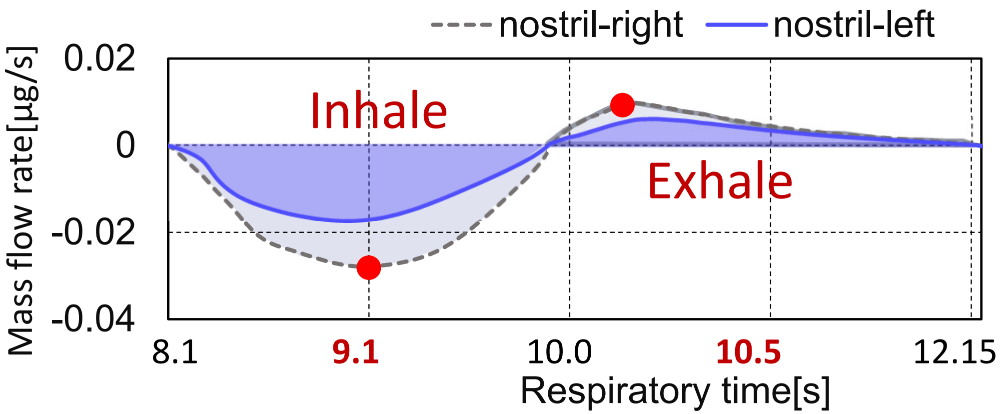


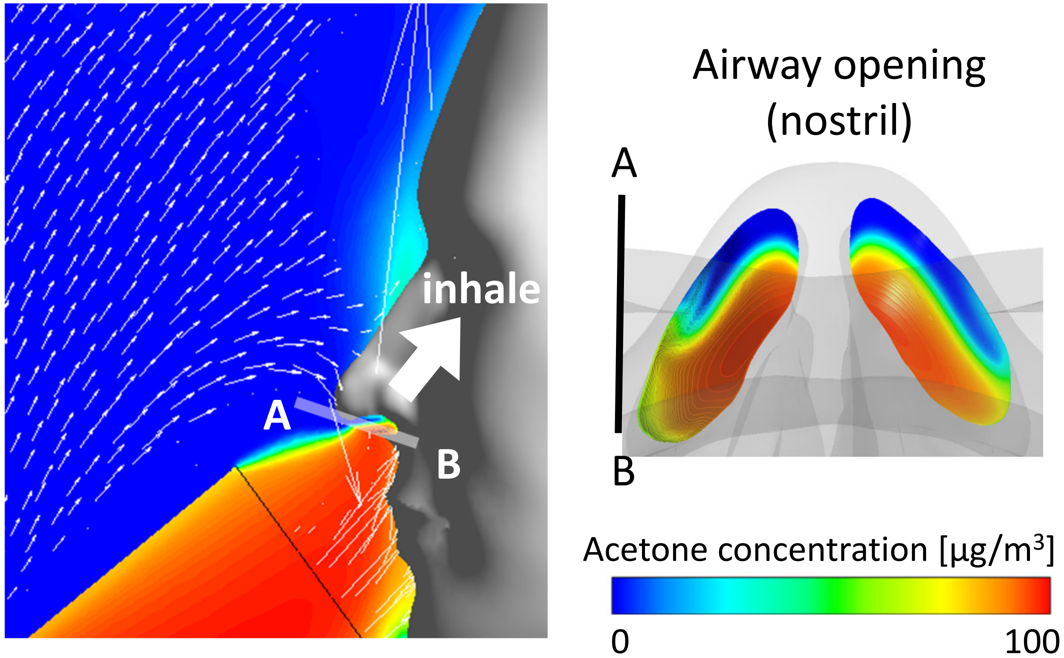
Transient *Acetone* Concentration Distribution



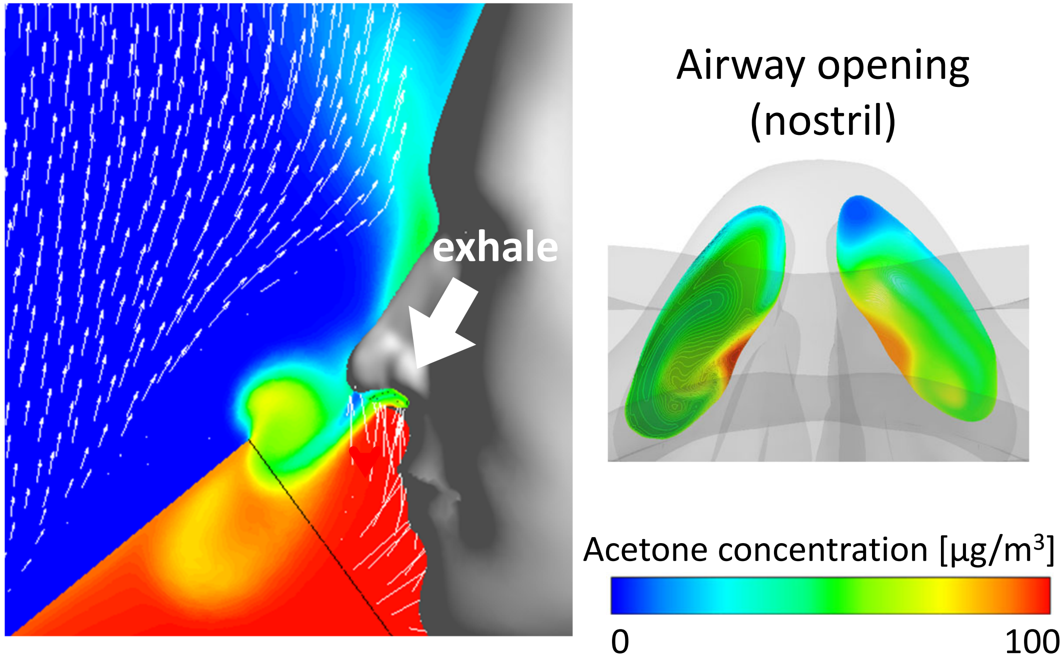
Center cross section of in Silico human (x=1.35m)

Inhaled/Exhaled *Acetone* Concentration via Right/Left-Nostril



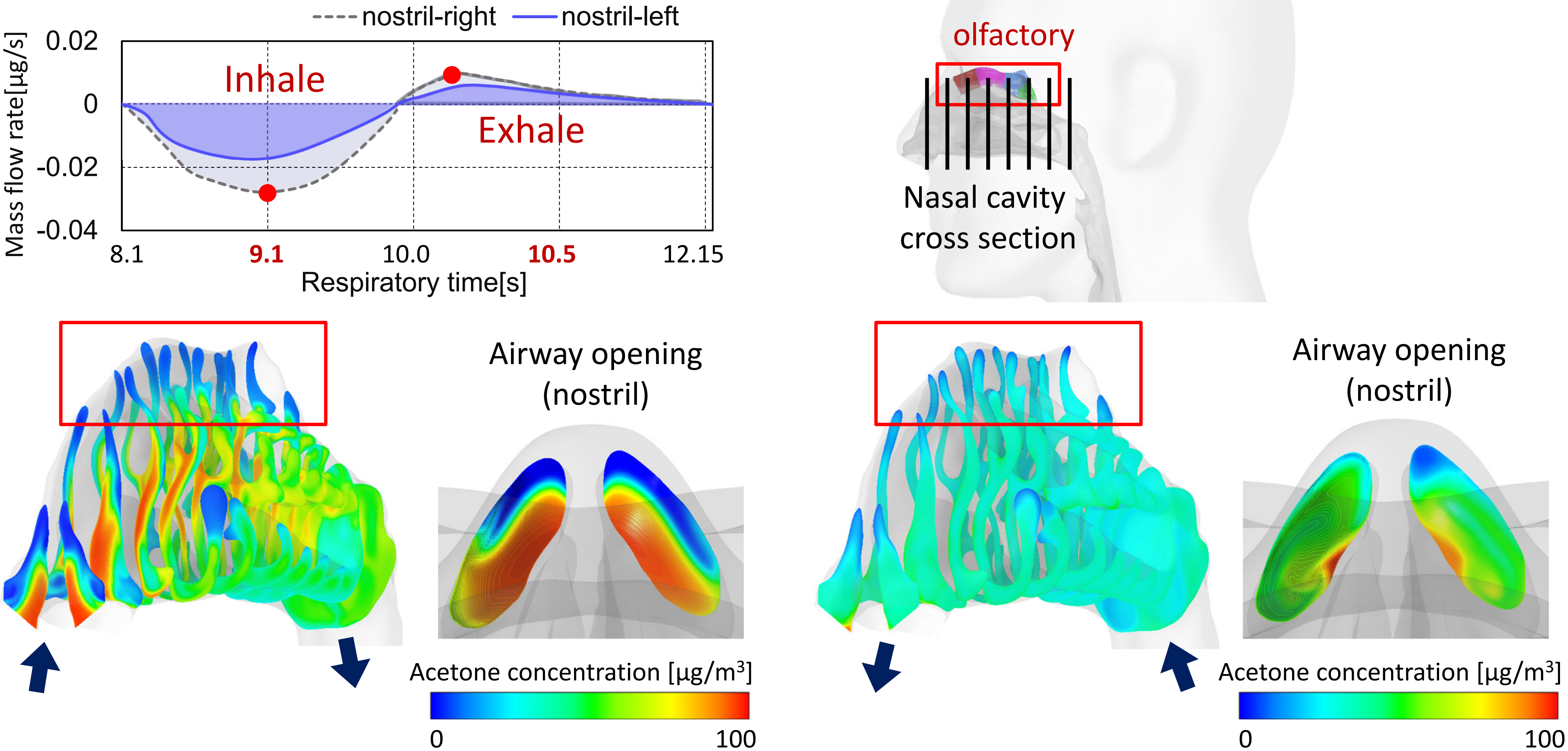


Inhale condition (9.1s)



Exhale condition (10.5s)

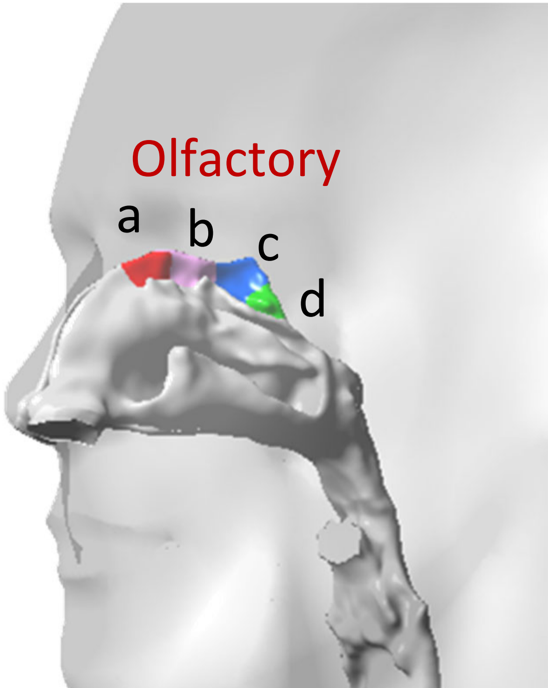
Acetone Concentration Distributions in Nasal Cavity



Inhale condition (9.1s)

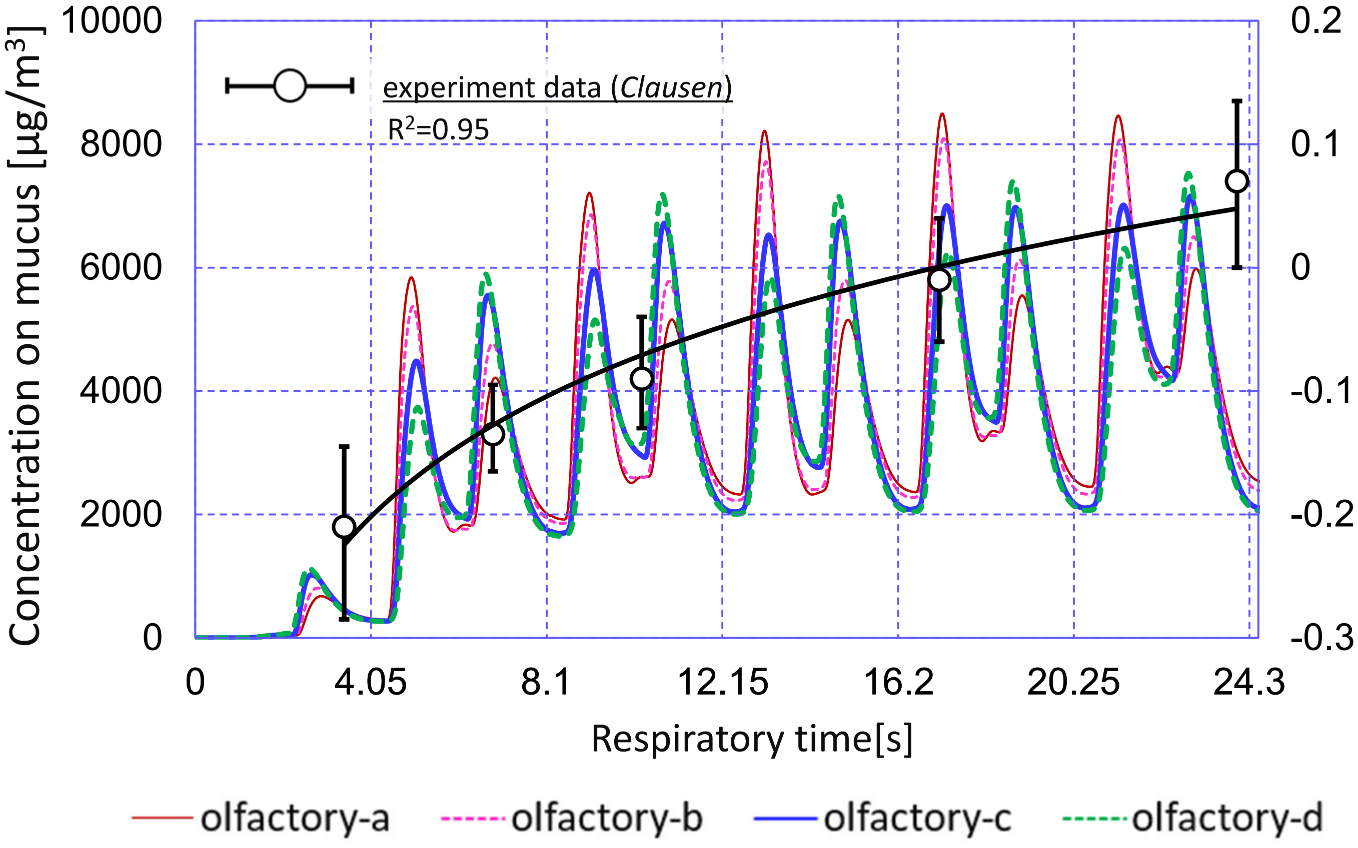
Exhale condition (10.5s)

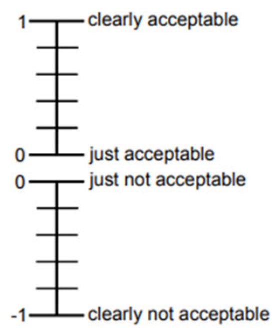
CFD-PBPK Analysis – *Acetone* concentration on mucus layer



Surface area [cm²]

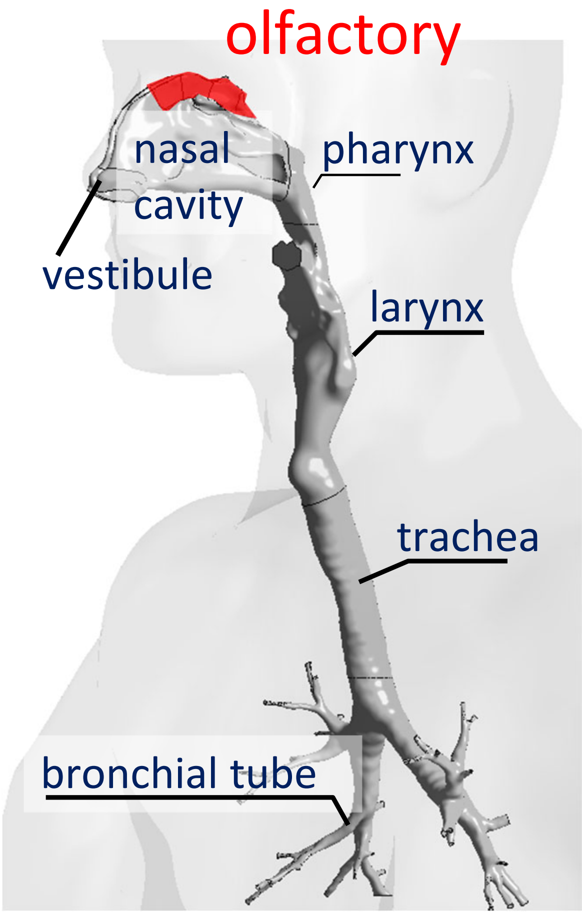
a	b	c	d
3.94	4.40	5.14	2.08

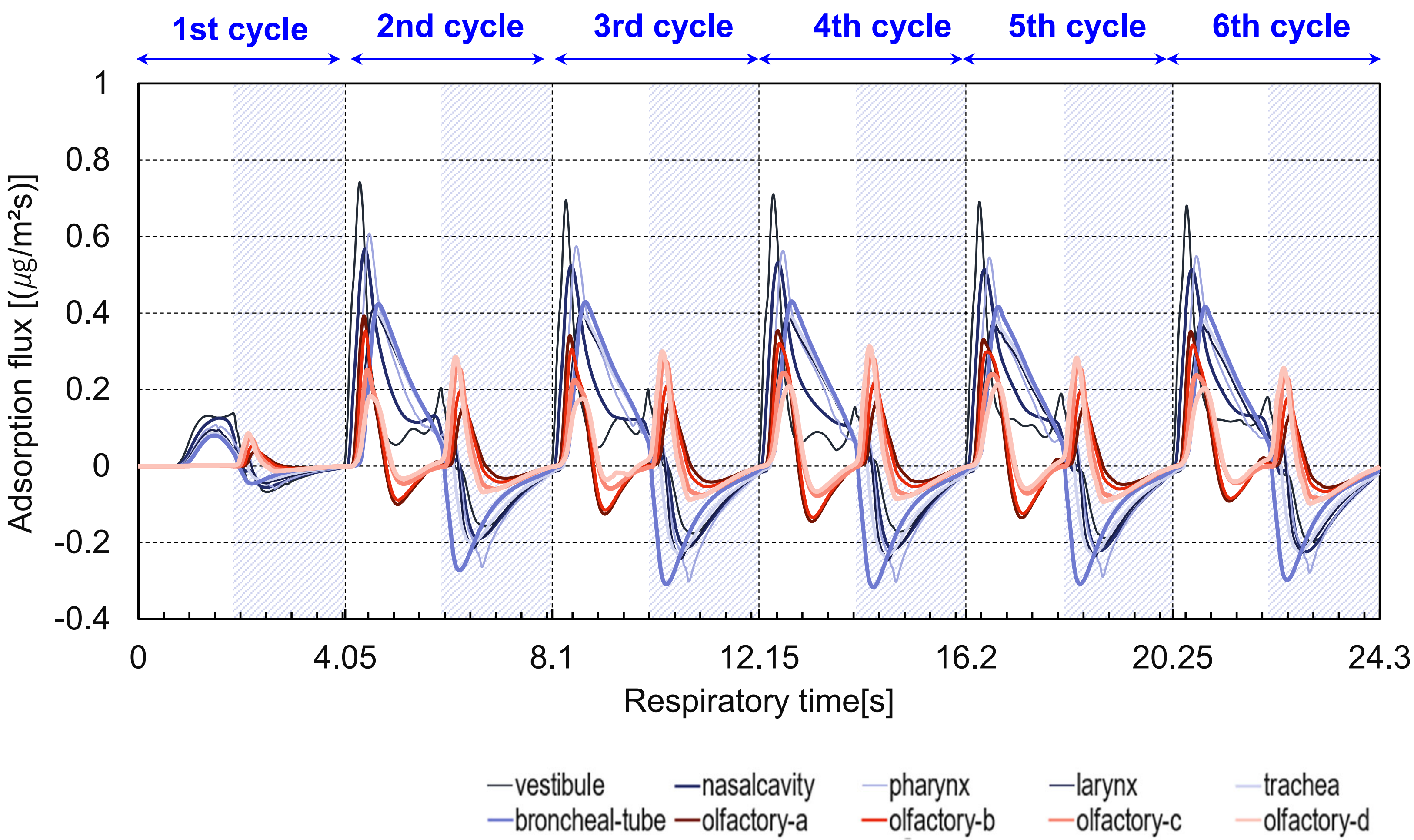




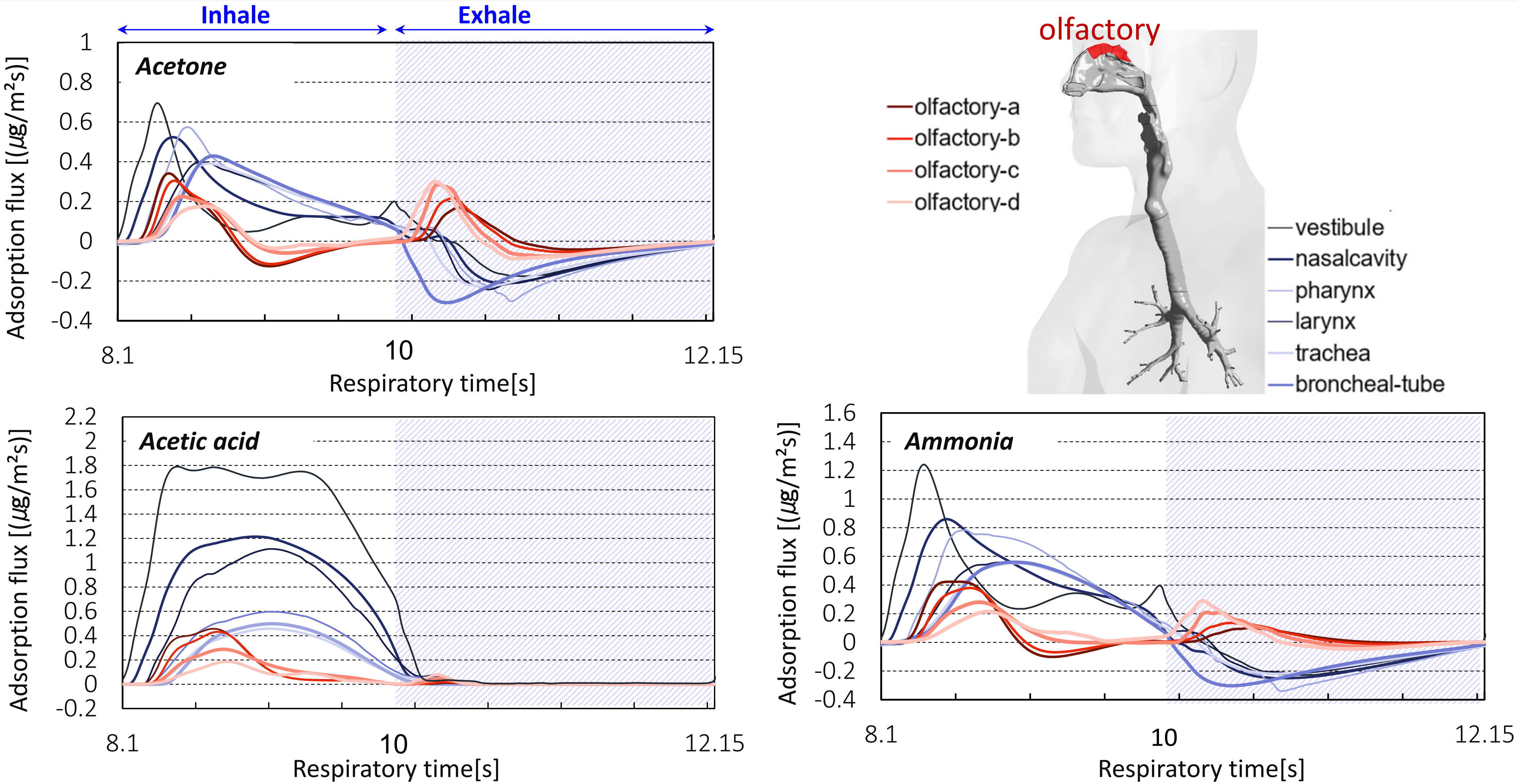
Clausen G (2000) Sensory evaluation of emissions and indoor air quality. In: Proceedings of healthy buildings 2000, vol 1, Espoo, pp 53–62

CFD-PBPK Analysis – *Acetone* Adsorption Flux on Mucus Surface

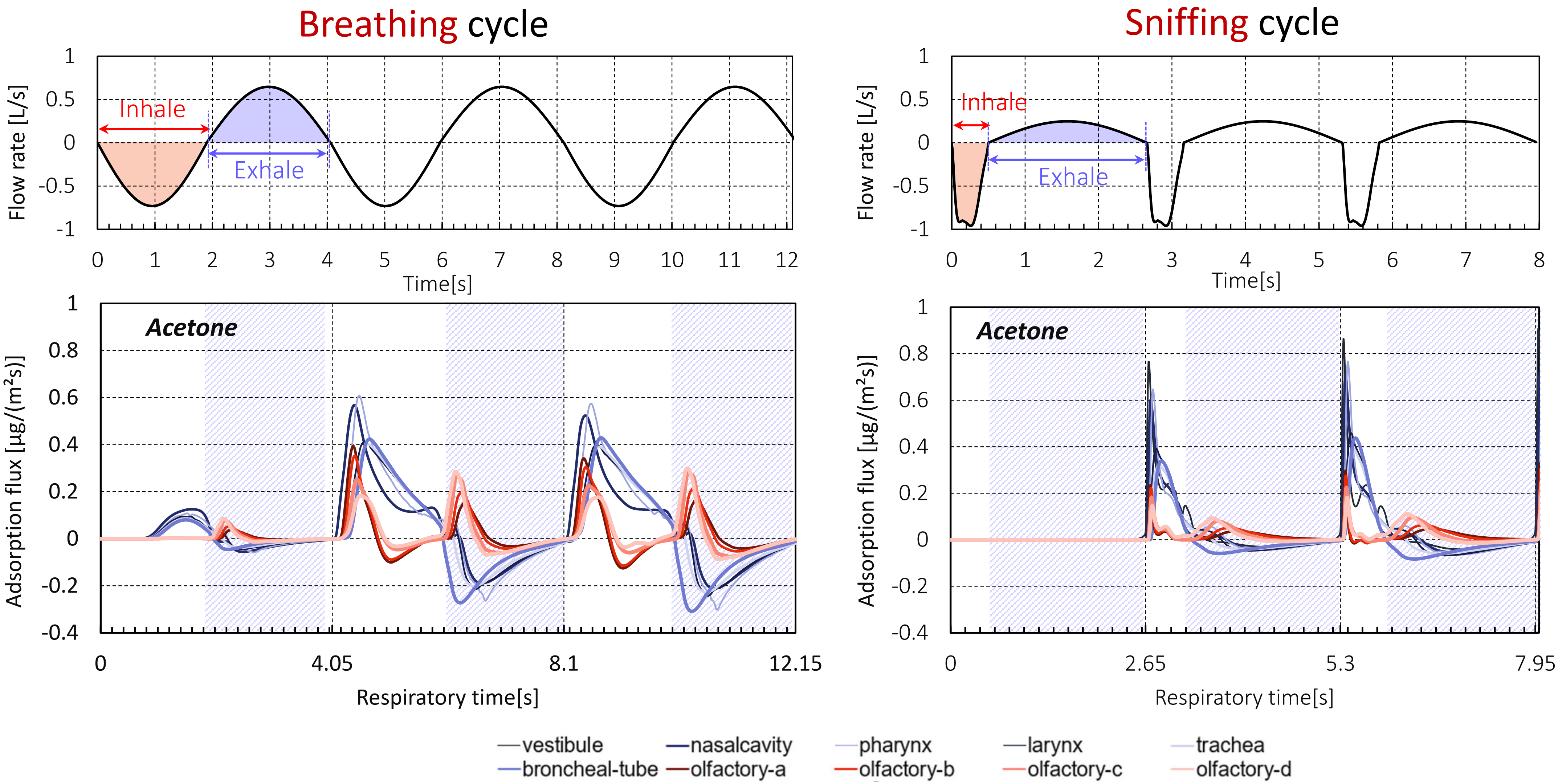




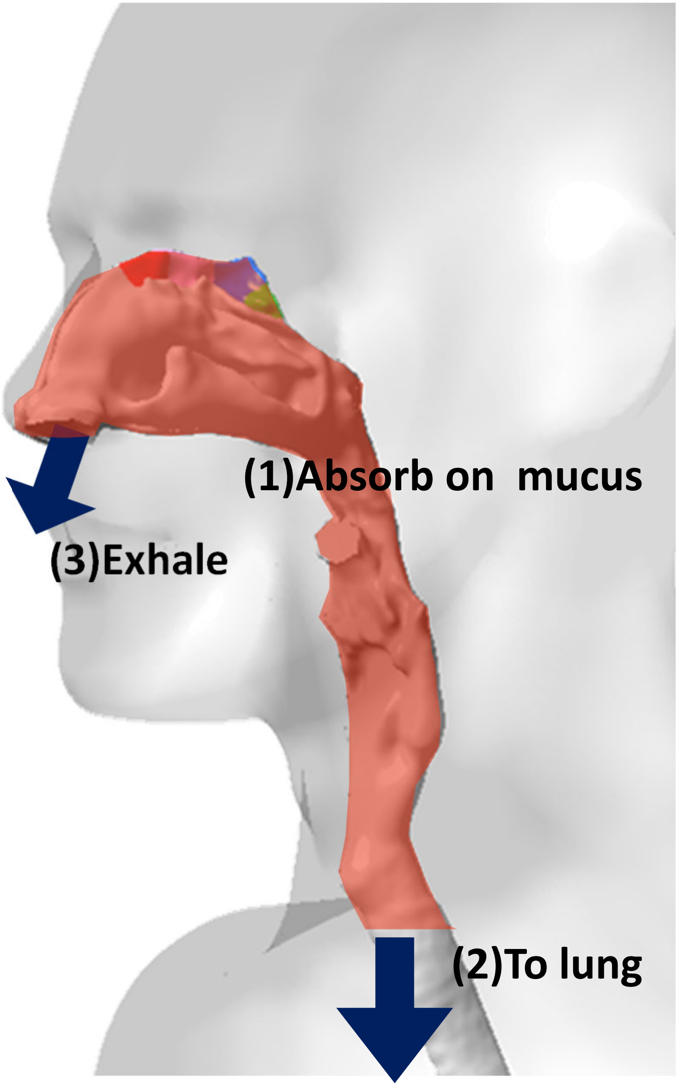
Adsorption Flux of *Acetone*, *Acetic acid*, and *Ammonia* on Mucus Surface

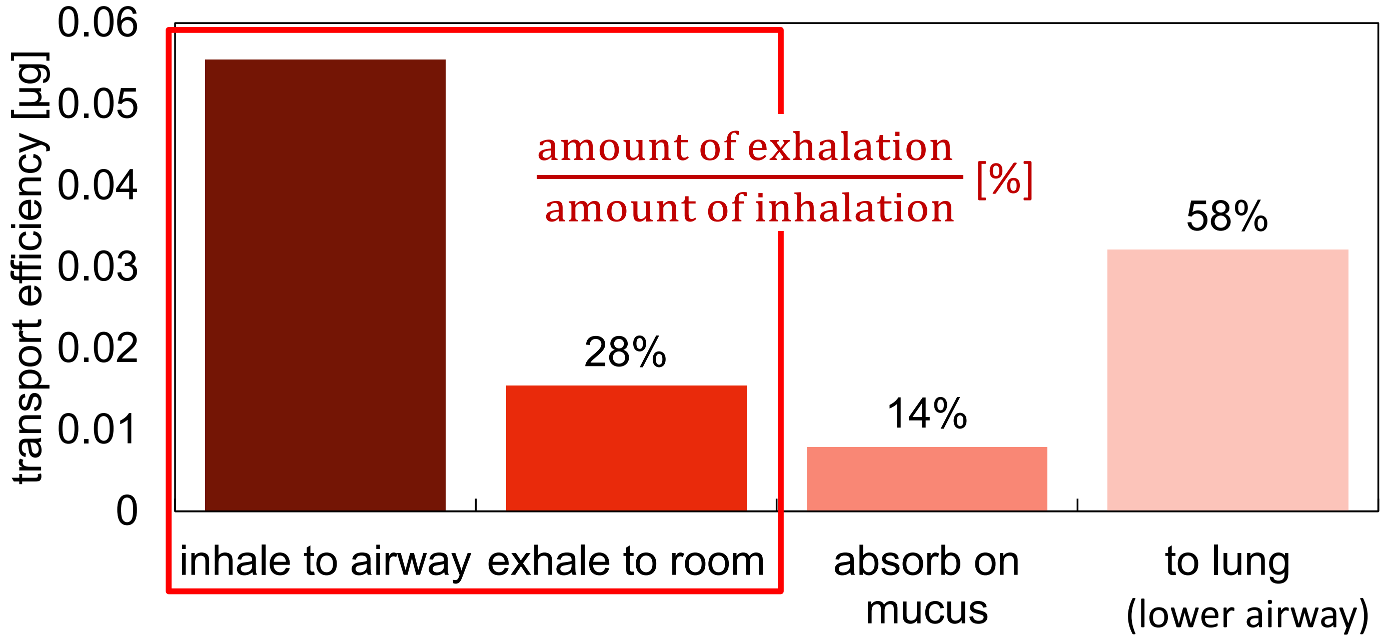


Breathing or Sniffing Cycle

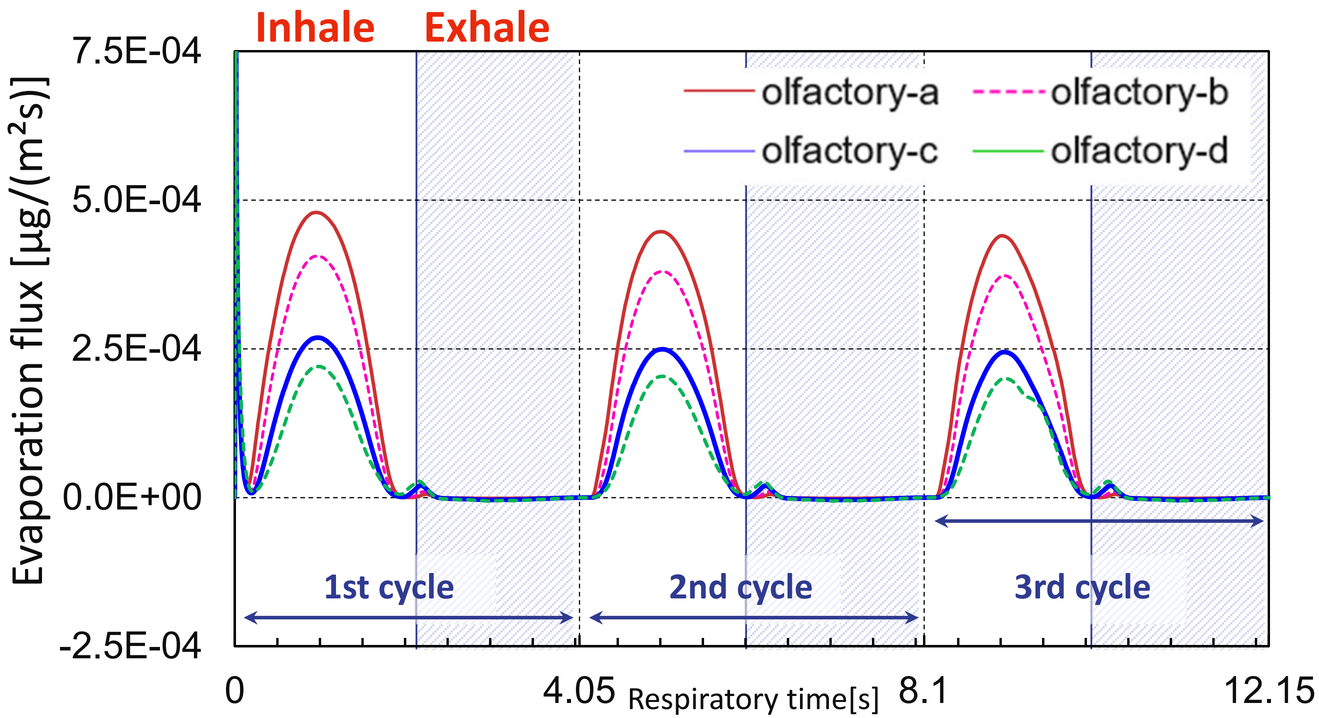


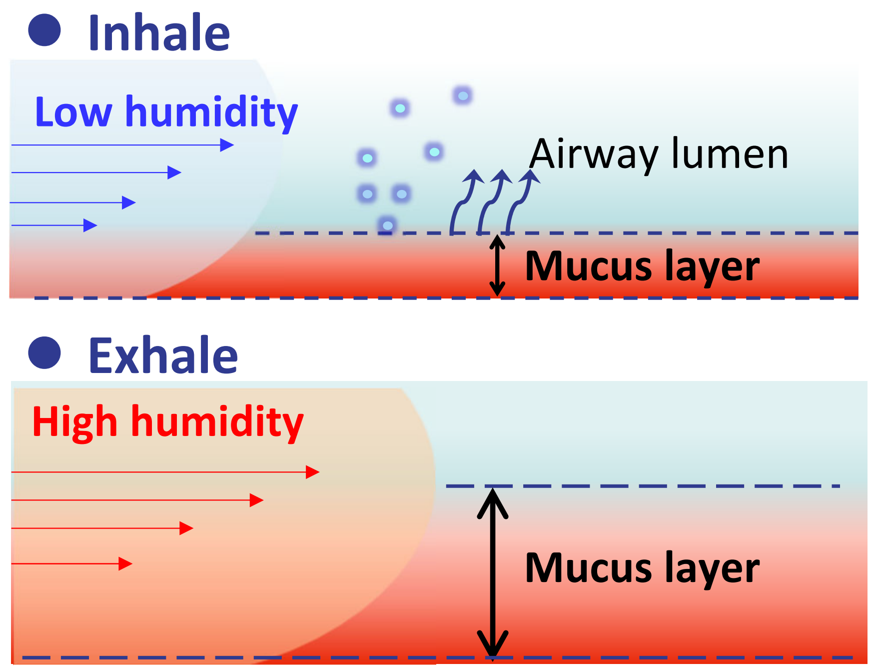
CFD-PBPK Analysis – Contribution Ratio of *Acetone* Distribution

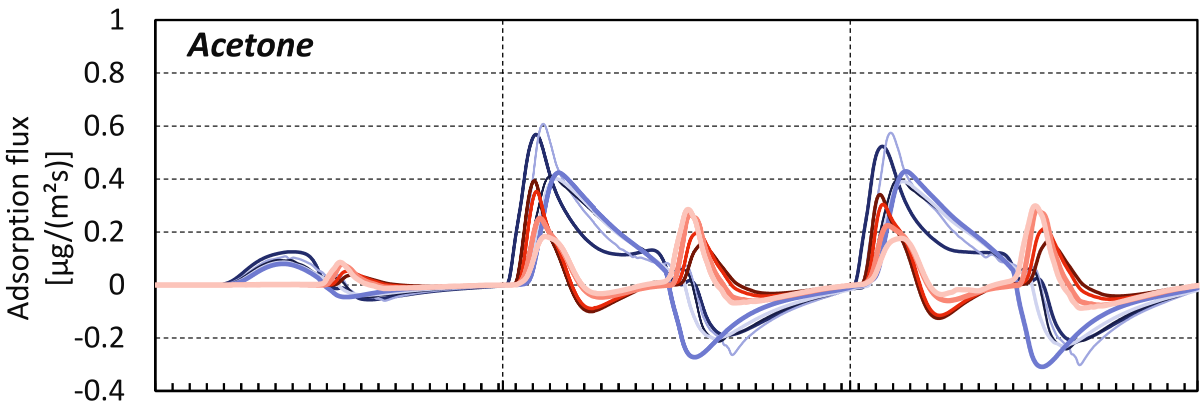




Hygrothermal Analysis – Evaporation flux on mucus surface

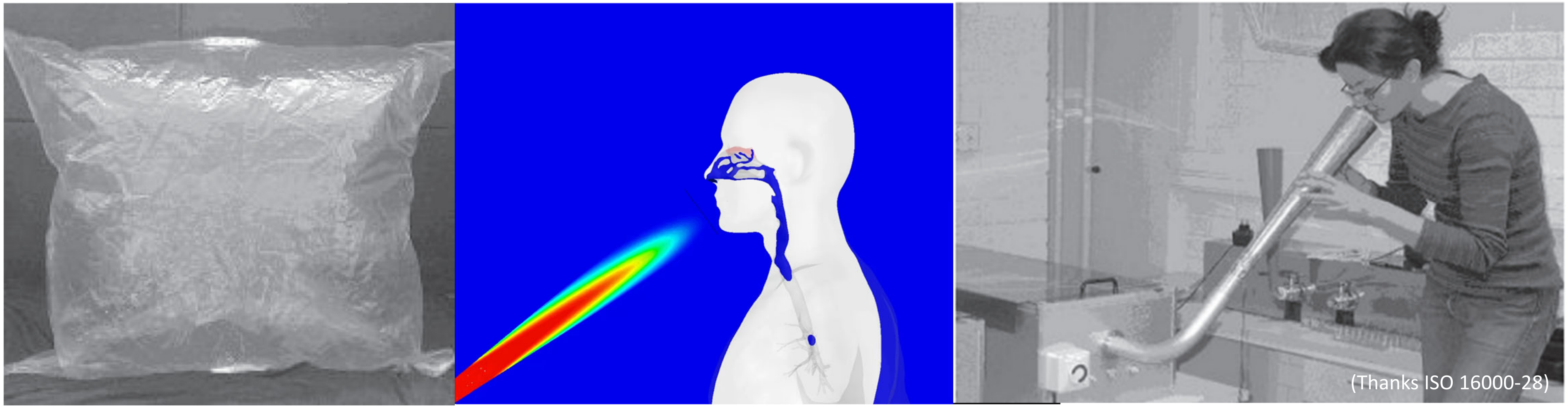






In Silico Human model or Volunteer Participants for Smell/ Odour Evaluation

- At present, adsorption flux (of chemical compounds) and sensible/latent heat flux to olfactory epithelial tissue may be analyzed quantitatively, but their combined effect on acceptability and perceived odour intensity evaluation could not be analyzed.
- Olfactory fatigue is also numerically unpredictable.
- Hence, still we do not know how many sniff/breath would be appropriate to odour evaluation.



(Thanks ISO 16000-28)