Identification of Appropriate CFD Models for Indoor Particle and Droplet Simulation in Ventilated Spaces

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Vent2006

Indoor Air Pollution

- Consequences
  - Respiratory illness, allergy, asthma (NIOSH 1999)
  - Sick building symptoms (SBS) (EPA 1991)
  - Productivity and economic losses (Fisk 2000)
- Causes
  - Gases: sulfur dioxide, carbon monoxide…
  - Particles: dusts, tobacco smoke…
  - Droplets: saliva, nasal droplets…

Typical Indoor Air Pollution Particle Sizes

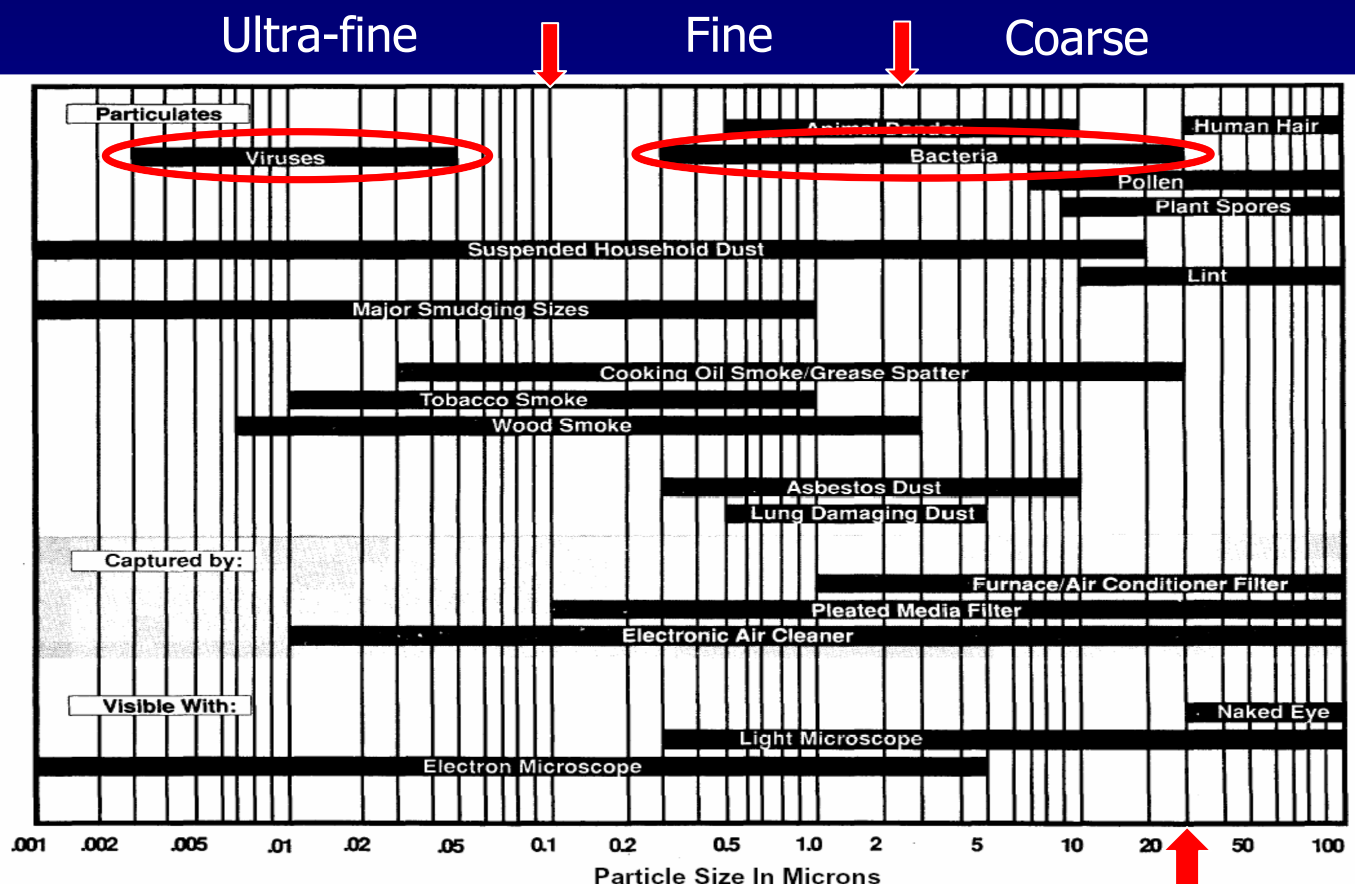
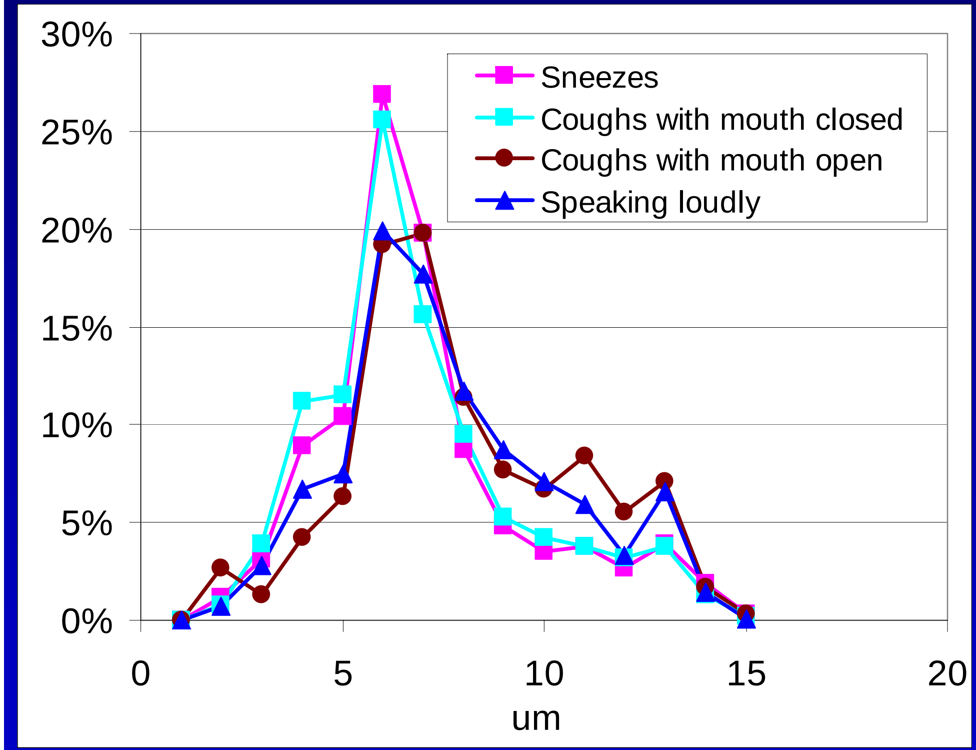


Figure 1. Size Ranges of Indoor Air Pollution Particles and Control Devices.

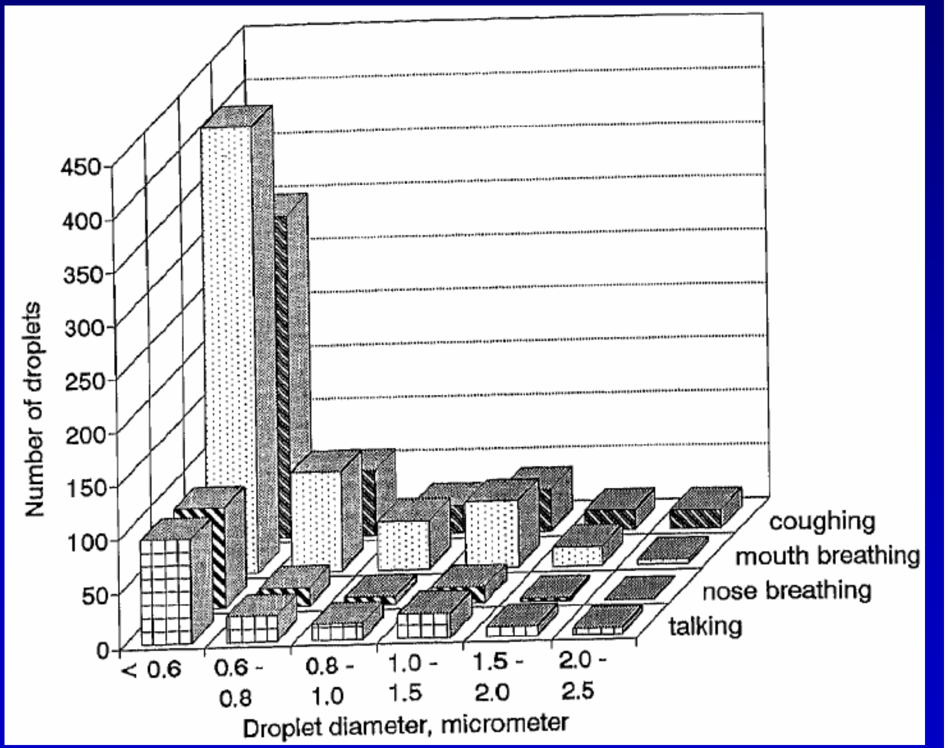
(Annis 1991)

400 million/ft^3 unseen particles

Typical Indoor Air Pollution Particle Sizes



(Duguid 1946)



(Papineni and Rosenthal 1997)

Popular CFD Models for Indoor Particle and Droplet Simulation

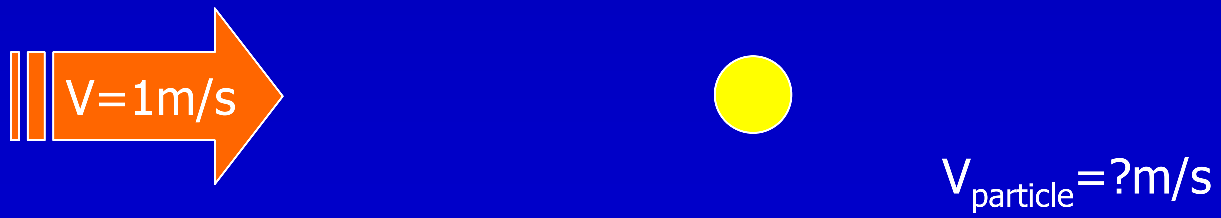
- Lazy particle model
- Isothermal particle model
- Vaporizing droplet model

Lazy Particle Model

- Share the continuous-phase velocity
- No size or temperature info
- Undergo no physical process (such as solidification or vaporization)
- No effect on the continuous phase
- Also called “tracer” model

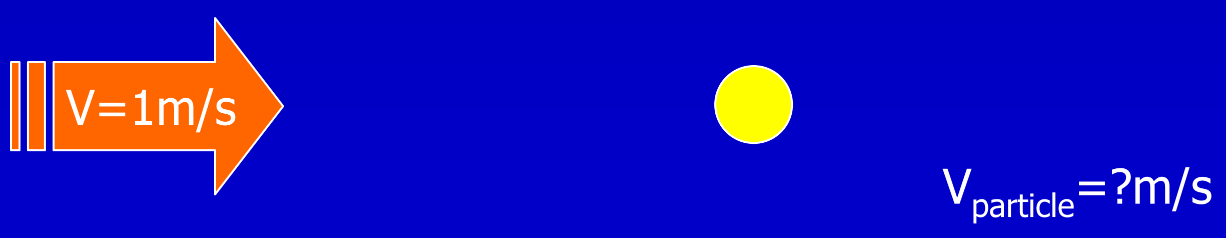
Isothermal Particle Model

- Particle position and velocity computed by Lagrangian particle transport equations
- Momentum transfer from air to particles
- No temperature or size change
- No exchange of heat or mass between air and particles

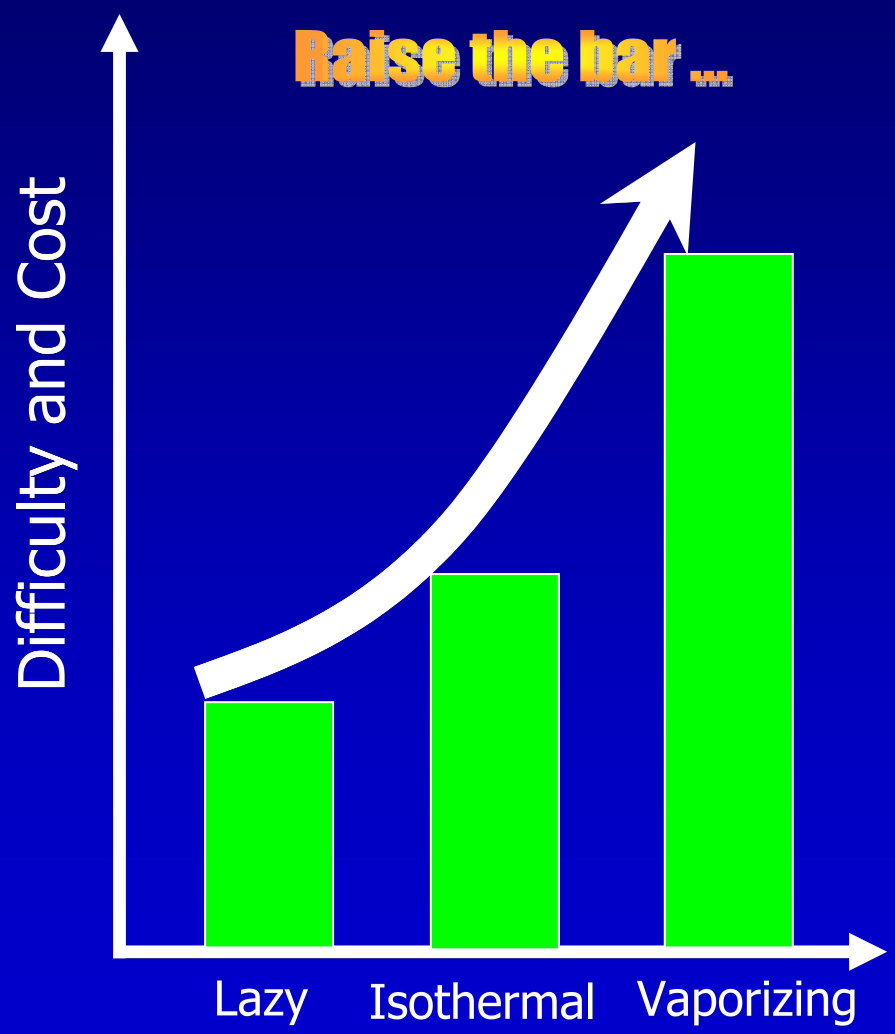


Vaporizing Droplet Model

- Particle position, velocity, temperature, and mass computed by Lagrangian droplet transport equations
- Exchange of momentum, enthalpy and mass between air and droplets



Which Model to Use ?



- Which model is most effective and efficient for a certain particle or droplet
- How large is the difference of results predicted by different models
- Factors:
  - Accuracy requirements
  - Computing cost
  - Particle size
  - Environment conditions

General Lagrangian Transport Equation For Particle and Droplet (1)

$$\frac{d(mv)}{dt} = \sum F = \frac{1}{2} C_D \frac{\pi D^2}{4} \rho_a \left(\vec{u} - \vec{v}\right)\left|\vec{u} - \vec{v}\right| + m\vec{g}$$

- Assumptions:
  - Sphere particle or droplet
  - Particles size above 1 μm (so Brownian force excluded)
  - Particle density on the order of 10^3 kg/m^3 or more (so unsteady forces and pressure gradient force excluded)
  - Sparse particle loading (the momentum effect of particles on air negligible)
- Momentum equation based on Newton's second law: only drag force and gravity force are included (Crowe et al. 1998)
  - *v=particle velocity; u=air velocity;* ρ_a*=air density; m=particle mass; D=particle diameter; g=gravitational acceleration;* C_D*=drag coefficient*

General Lagrangian Transport Equation For Particle and Droplet (2)

Introducing the particle Reynolds number Re_r and drag factor f

$$Re_r = \frac{\rho_a D \left|\vec{u} - \vec{v}\right|}{\mu_a} \qquad f = \frac{C_D \, Re_r}{24}$$

$$\frac{d\vec{v}}{dt} = \frac{18\mu_a}{\rho_p D^2} \frac{C_D \, Re_r}{24} \left(\vec{u} - \vec{v}\right) + \vec{g} = \frac{18\mu_a}{\rho_p D^2} f \left(\vec{u} - \vec{v}\right) + \vec{g}$$

v=particle velocity; u=air velocity; ρ_a=air density; μ_a=air viscosity; D=particle diameter; ρ_p=particle density; g=gravitational acceleration; C_D=drag coefficient

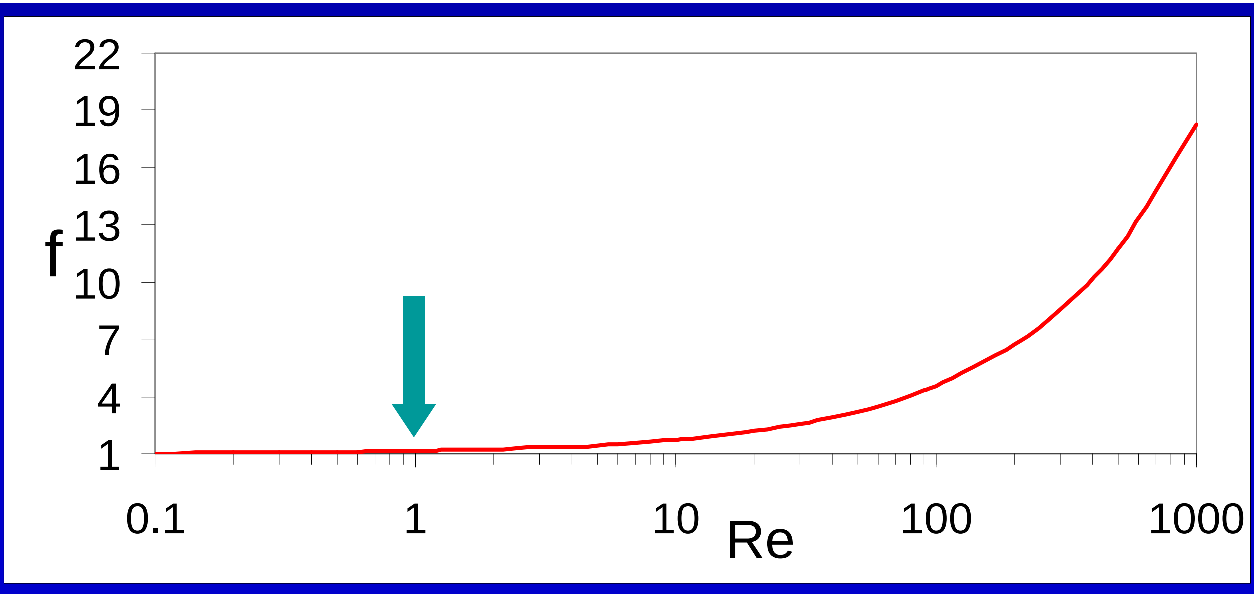
General Lagrangian Transport Equation For Particle and Droplet (3)

Particle and Droplet Transport Equation to Be Solved

$$\frac{d\vec{v}}{dt} = \frac{18\mu_a}{\rho_p D^2} f\left(\vec{u} - \vec{v}\right) + \vec{g}$$

Clift and Gauvin (1970)

$$f = 1 + 0.15\,\mathrm{Re}_r^{0.687} + 0.0175 \times \left(1 + 4.25 \times 10^4\,\mathrm{Re}_r^{-1.16}\right)^{-1}$$



Analysis of Low Reynolds Particle Flow
(Re_r<1) (Stokes Flow)

$$\frac{d\vec{v}}{dt} = \frac{\left(\vec{u} - \vec{v}\right)}{\tau_v} + \vec{g}$$

$$\tau_v = \frac{\rho_p D^2}{18\mu_a}$$

is defined as the particle momentum (velocity) response time

2-D Cases

$$\frac{dv_x}{dt} = \frac{u_x - v_x}{\tau_v}$$

$$\frac{dv_y}{dt} = \frac{u_y - v_y}{\tau_v} - g$$

Solutions

for constant D and U and V(t=0)=0

$$v_x = u_x\left(1 - e^{-t/\tau_v}\right)$$

$$v_y = \left(u_y - \tau_v g\right)\left(1 - e^{-t/\tau_v}\right)$$

Analysis of Low Reynolds Particle Flow
(Re_r<1) (Stokes Flow)

If t=infinite

$$v_x = u_x$$

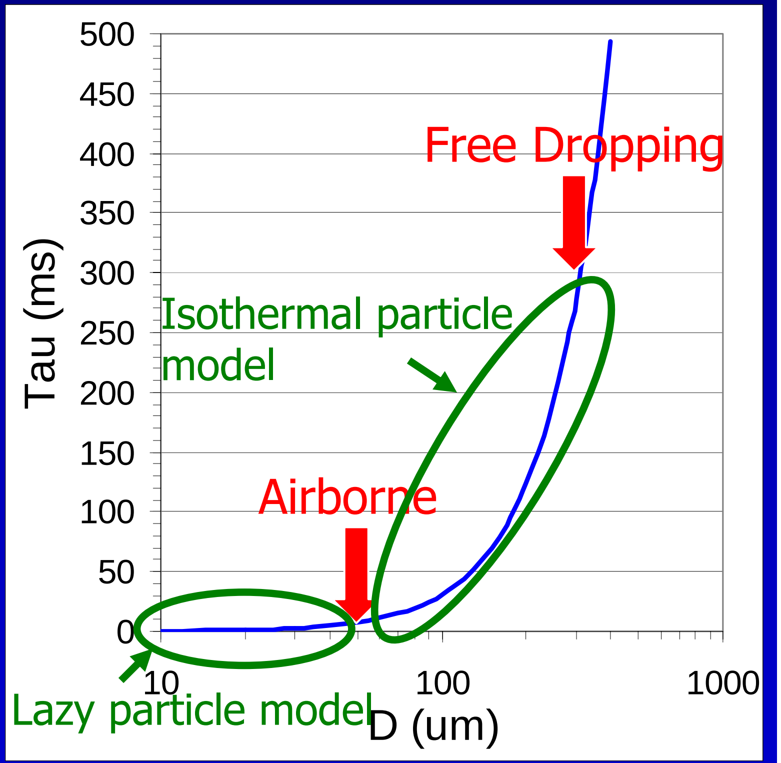
$$v_y = (u_y - \tau_v g)$$

If t=τ_v

$$v_x = 63\% \cdot u_x$$

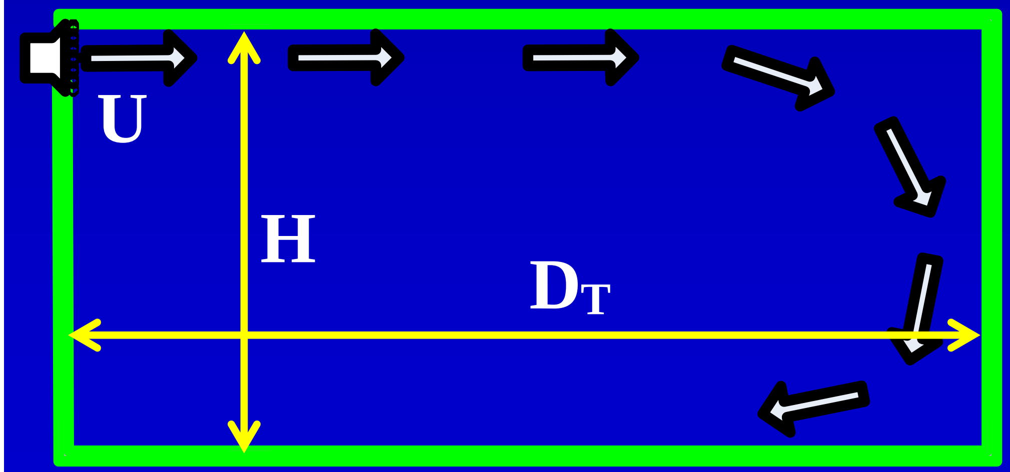
$$v_y = 63\% \cdot (u_y - \tau_v g)$$

So, the particle momentum response time τ_v indicates how fast the particle can reach the air velocity and respond to the air velocity changes.



Analysis of Low Reynolds Particle Flow (Re_r<1) (Stokes Flow)

- Definition: Stokes Number $St_v = \frac{\tau_v}{\tau_F}$
- τ_F is the characteristic time of a flow field that represents the shortest time for certain particle to be caught by obstructions.
- Definition: $\tau_F = \min\left(D_T/U, \sqrt{2H/g}\right)$



Stokes Number	Category
St_v<<1	Lazy particle
$St_v \approx$ 1	Isothermal particle
St_v>>1	Free dropping particle

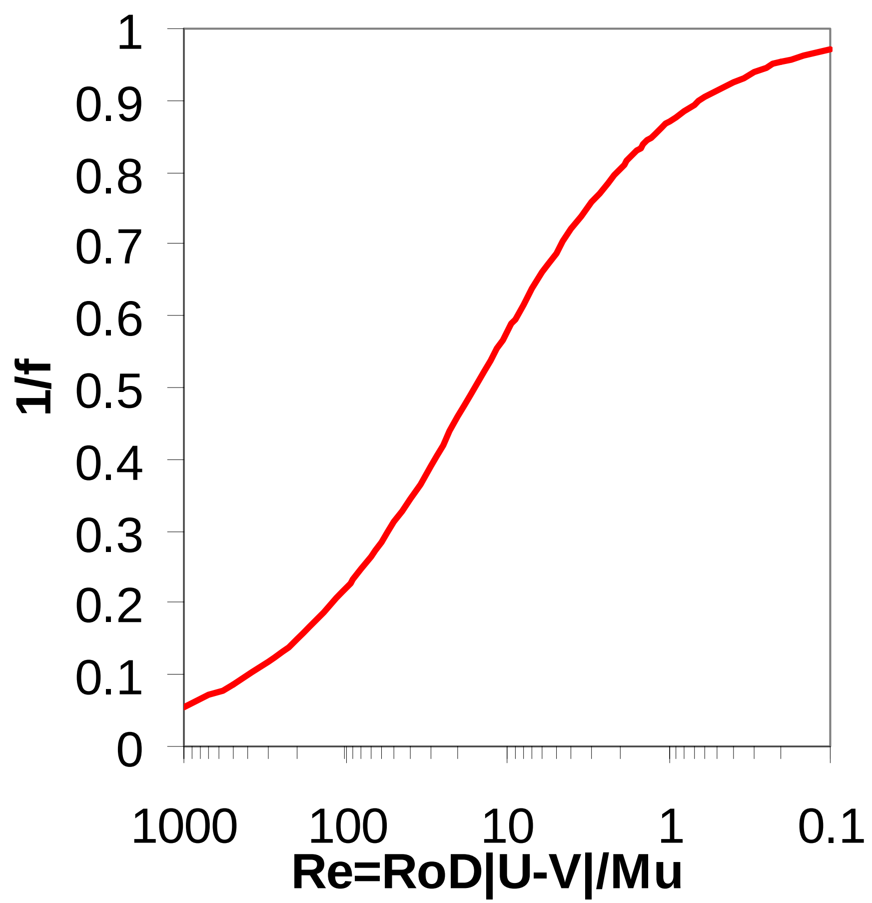
Analysis of High Reynolds Particle Flow ($Re_r > 1$)

$Re_r > 1 \Rightarrow f > 1$ and $f = F(Re_r)$

$$\frac{d\vec{v}}{dt} = \frac{\left(\vec{u} - \vec{v}\right)}{\tau'_v} + \vec{g}$$

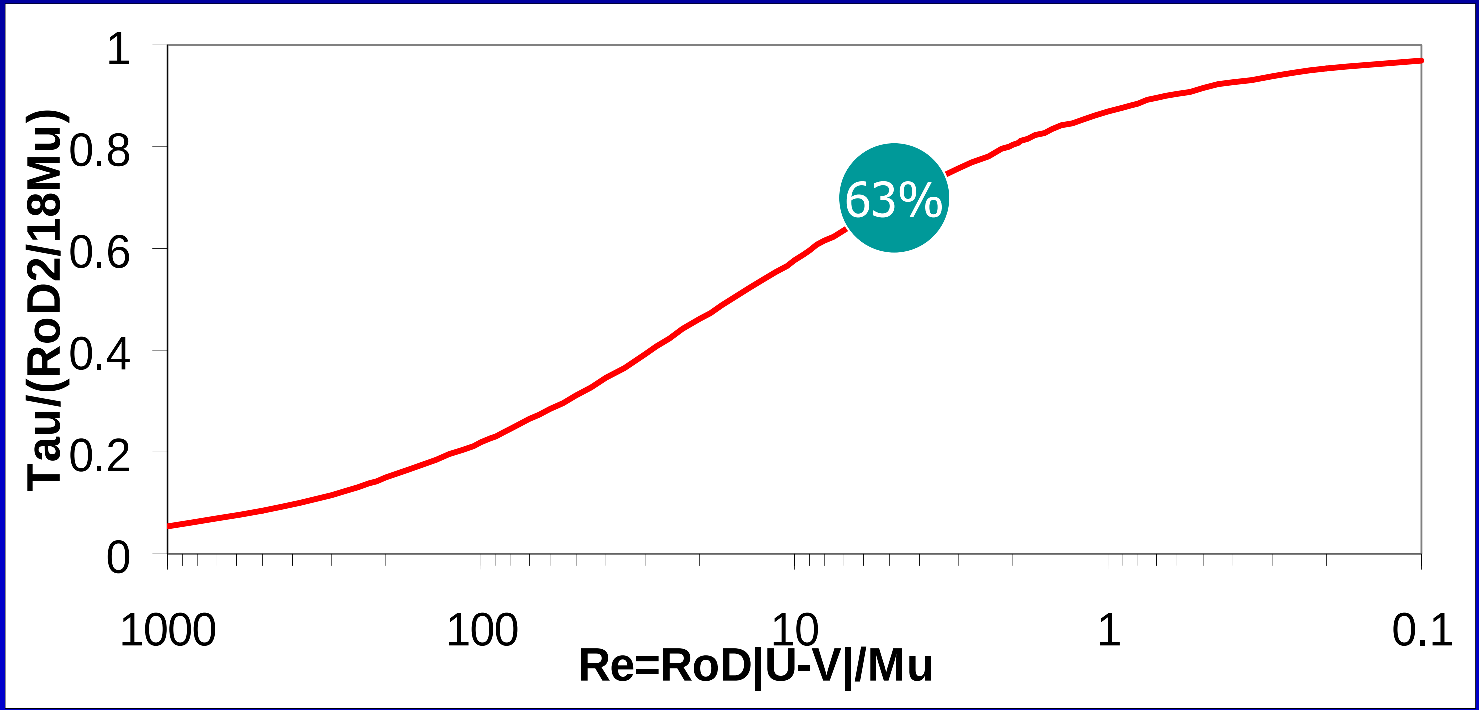
$$\tau'_v = \frac{\rho_p D^2}{18\mu_a} \frac{1}{f}$$

is defined as the modified particle momentum (velocity) response time



Analysis of High Reynolds Particle Flow (Re_r>1)

- $\tau'_{V=63\%U}$ estimates the time for a particle released from rest to achieve 63% of the free stream velocity.
- $\tau'_{V=63\%U}$ overestimates the real time but reflects its magnitude.



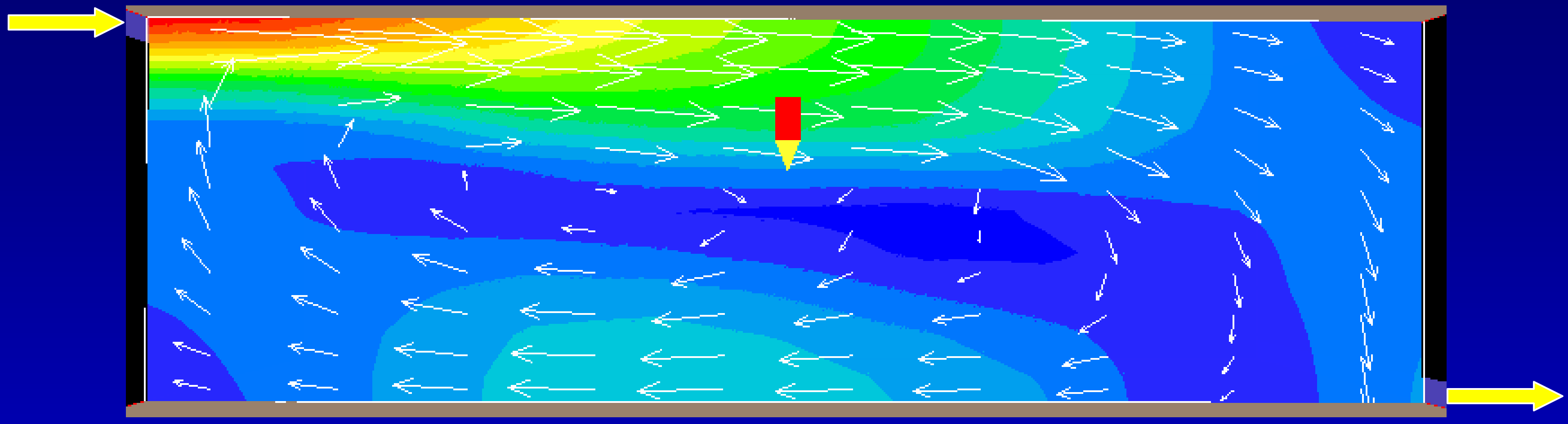
Analysis of High Reynolds Particle Flow
($Re_r>1$)

Stokes Number:

$$St_v = \frac{\tau'_{V=63\%U}}{\tau_F} \qquad \tau_F = \min\left(D_T/U, \sqrt{2H/g}\right)$$

Stokes Number	Category
$St_v<<1$	Lazy particle
$St_v\approx 1$	Isothermal particle
$St_v>>1$	Free dropping particle

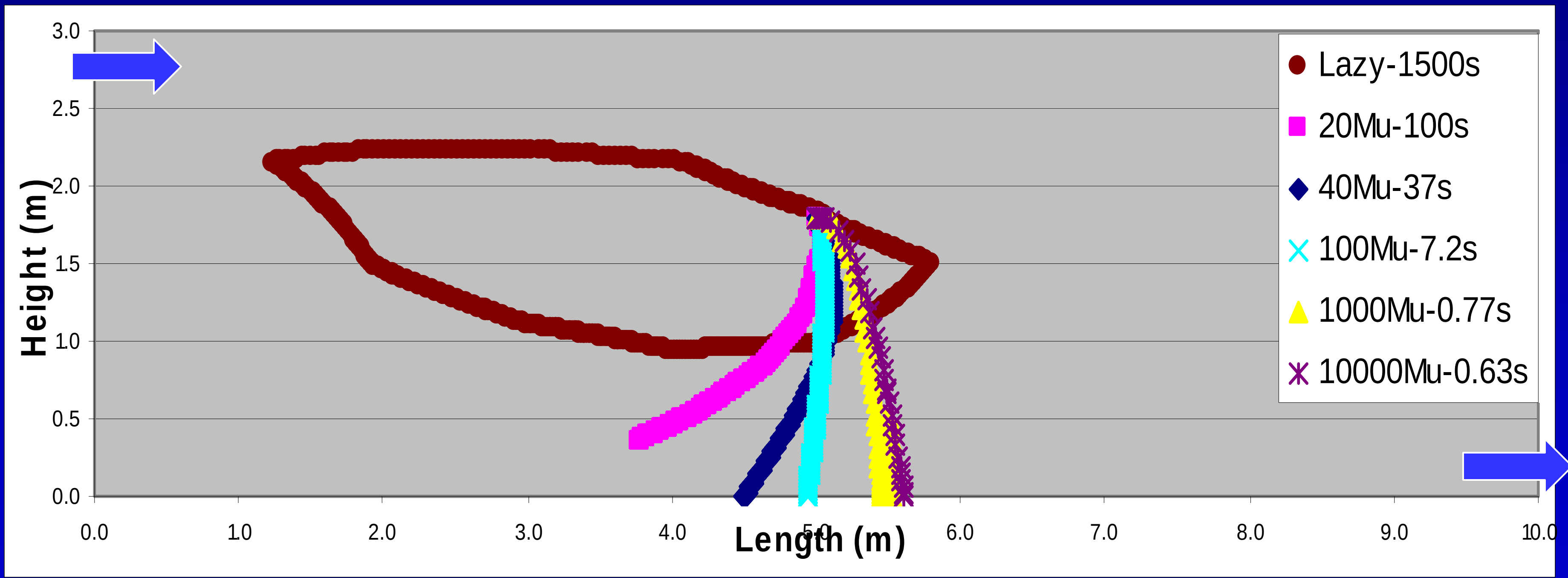
CFD Experiment of Air-Particle Models



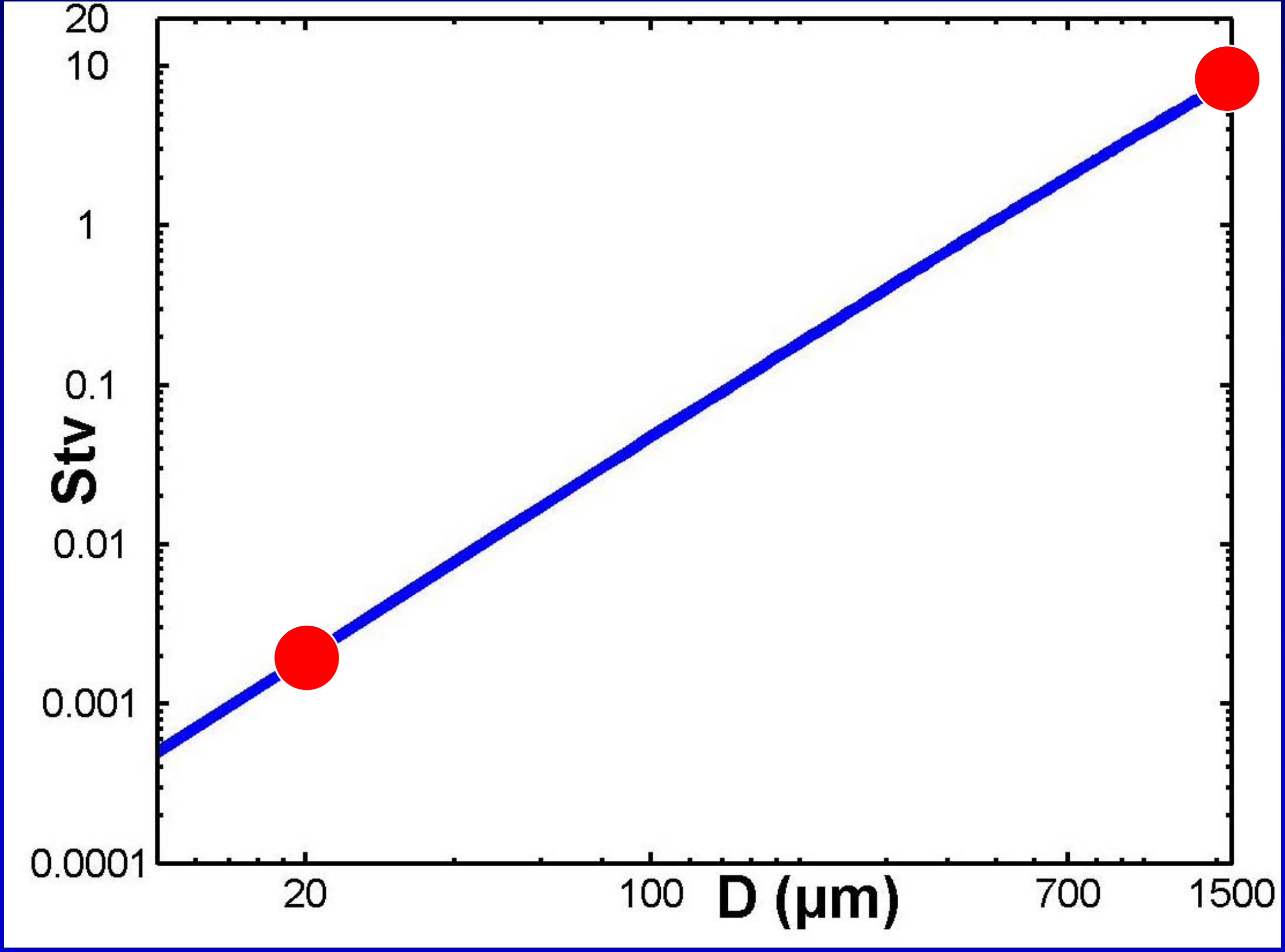
- 2D Room with Length=10m and Height=3m
- Inlet air velocity = 0.1m/s
- Solid particle released from the center of the room at height=1.8m (nose level)
- Flow characteristic time = 0.6s, which is the dropping time of a free object from 1.8m

CFD Experiment of Air-Particle Models

Trajectory of isothermal particles from CFD



CFD Experiment of Air-Particle Models



CFD Experiment of Air-Particle Models
(for both $Re_r>1$ and $Re_r>1$)

Stokes Number	**Category**	**Critical St_v**	**Corresponding D**
$St_v<<1$	Lazy particle	$St_{v,cr}=0.001$	$D_{cr}=20\mu m$
$St_v \approx 1$	Isothermal particle	$0.001<St_{v,cr}<10$	$20\mu m<D<1500\mu m$
$St_v>>1$	Free dropping particle	$St_{v,cr}=10$	$D_{cr}=1500\mu m$

Note: The corresponding D is calculated with typical building parameters:

$D_T=10m$, $H=3m$, $U=0.1m/s$, $\rho_p=1000kg/m^3$

Analysis of Droplet Flow in the Air

- Droplet Momentum Equation

$$\frac{d\vec{v}}{dt} = \frac{18\mu_a}{\rho_p D^2} f\left(\vec{u} - \vec{v}\right) + \vec{g}$$

- Droplet Mass Equation Due to Evaporation (Ludwig et al. 2004)

$$\frac{dm_p}{dt} = -\pi D_p \frac{K_v}{Cp_v} Nu \ln\left(1 + B_m\right)$$

Or $$D_p \frac{dD_p}{dt} = -2 \frac{K_v}{Cp_v} \frac{Nu}{\rho_p} \ln\left(1 + B_m\right)$$

m_p=droplet mass; D_p=droplet diameter; K_v=thermal conductivity of droplet vapor; Cp_v=specific heat capacity of droplet vapor; ρ_p=particle density; Nu=Nusselt number=$2(1+0.3Re^{0.5}Pr^{0.33})F$; Re=$D_p\rho_a |u-v|/\mu_a$; Pr=laminar Prandtl number of air; F=Frossling correction for mass transfer=$\ln(1+B_m)/B_m$; B_m=mass transfer number that is a function of vapor mass fraction at droplet surface and in the air

Analysis of Droplet Flow in the Air

$$D_p \frac{dD_p}{dt} = -2 \frac{K_v}{Cp_v} \frac{Nu}{\rho_p} \ln(1 + B_m) \approx \text{constant}$$

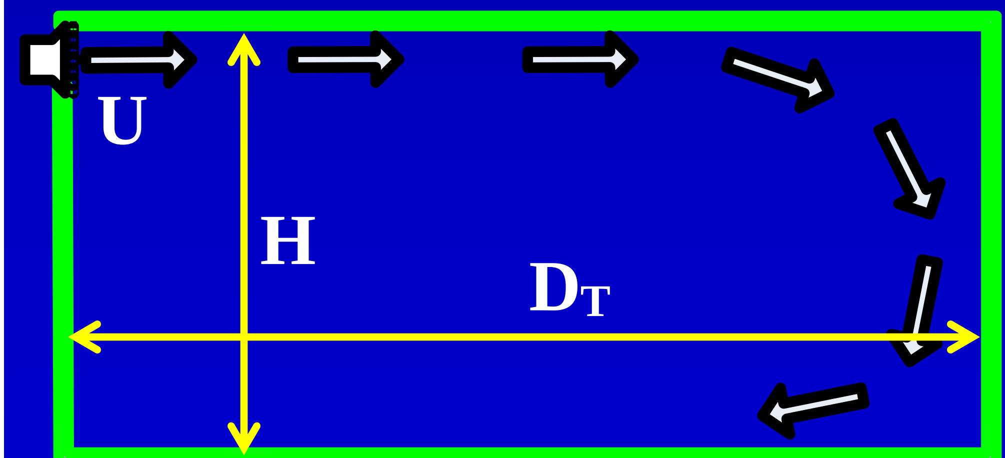
$$\Rightarrow \quad D^2 = D_0^2 - \lambda t$$

$$\lambda = 4 \frac{K_v}{Cp_v} \frac{Nu}{\rho_p} \ln(1 + B_m)$$

$$\Rightarrow \quad \tau_m = \frac{D_0^2}{\lambda}$$ Evaporation Lifetime

Analysis of Droplet Flow in the Air

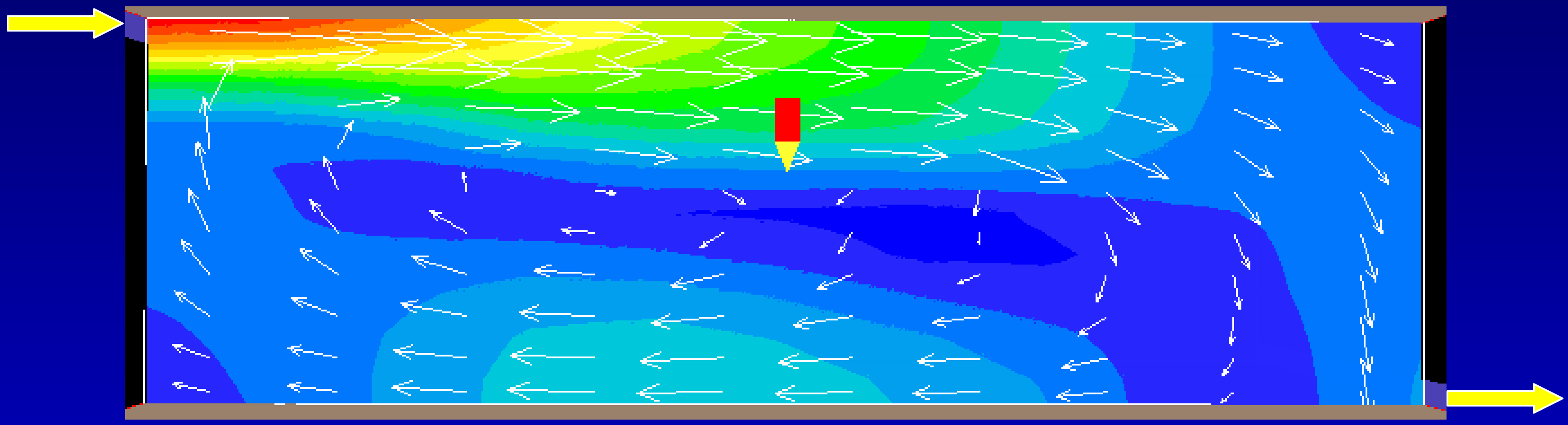
- Definition: Evaporation Effectiveness Number $EE = \frac{\tau_m}{\tau_F} = \frac{D_0^2}{\lambda \tau_F}$
- τ_F is the characteristic time of a flow field that represents the shortest time for certain particle to be caught by obstructions.
- Definition: $\tau_F = \min\left(D_T/U, \sqrt{2H/g}\right)$

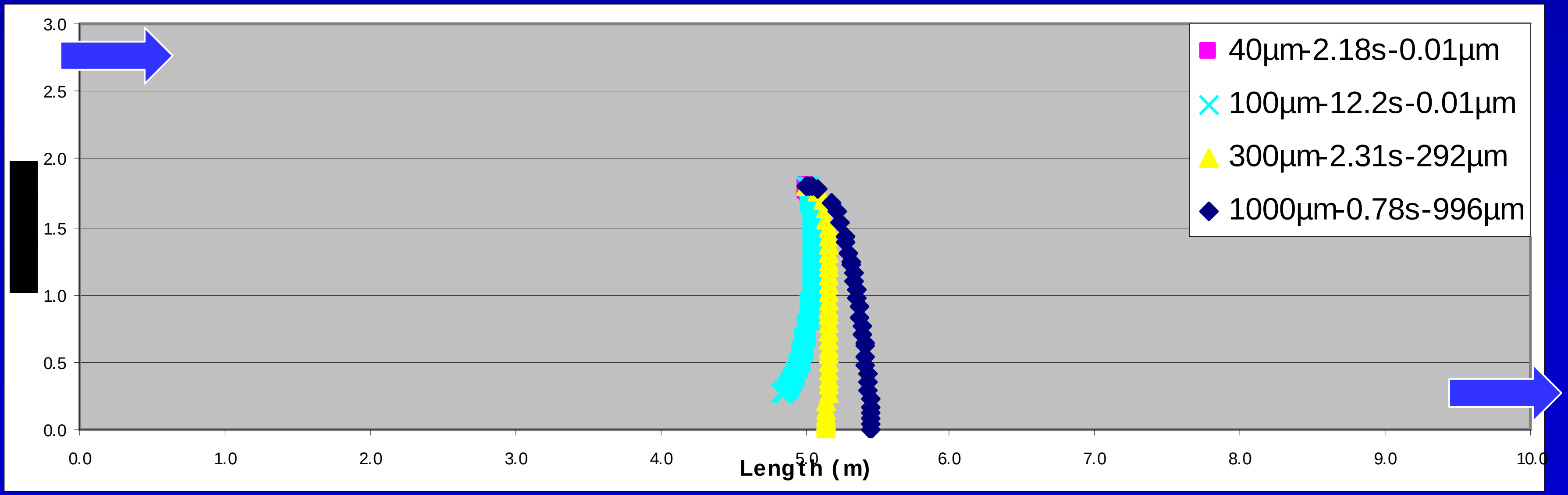


EE	Category
EE<<1	Lazy particle
EE≈ 1	Vaporizing particle
EE>>1	Isothermal particle

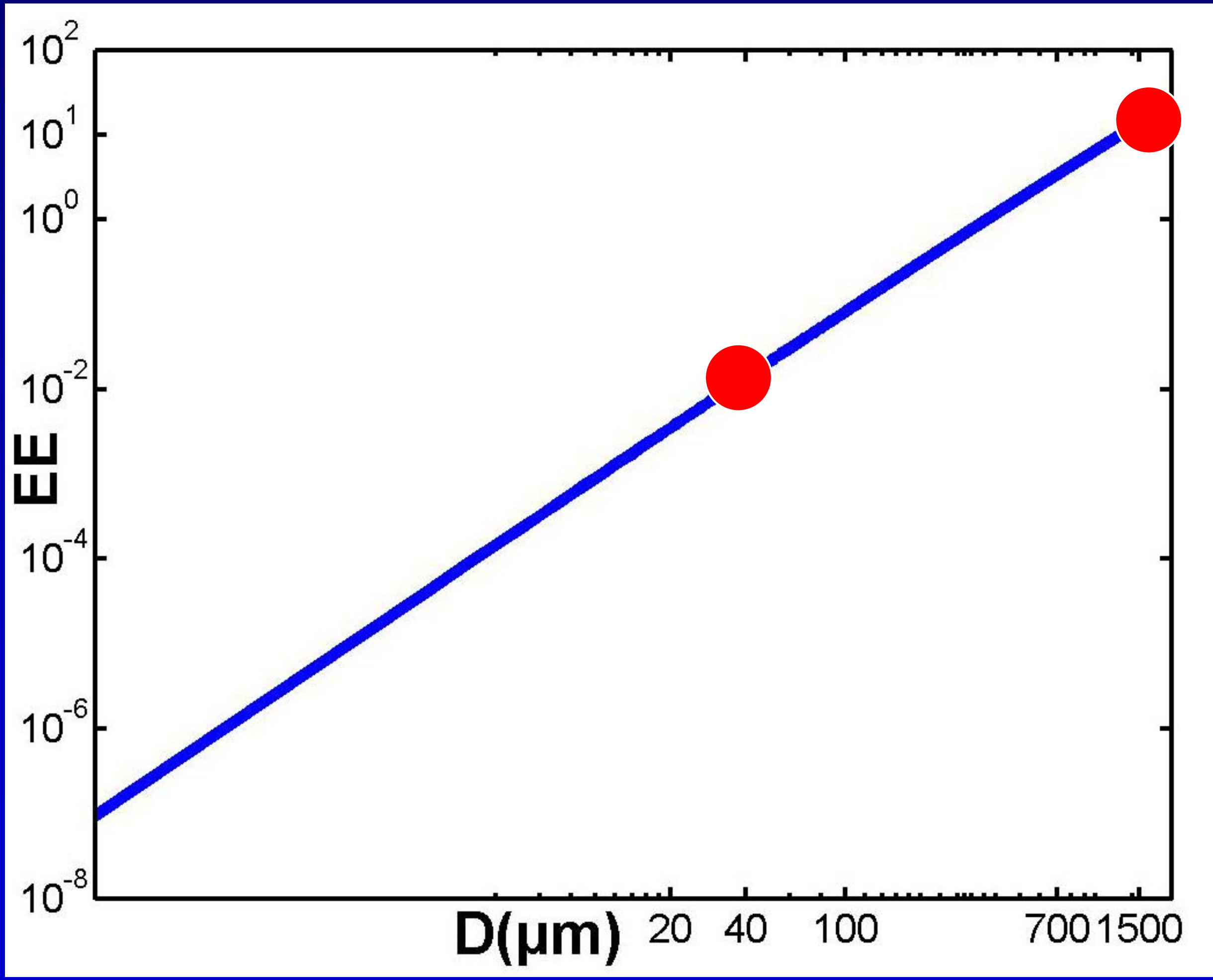
CFD Experiment of Air-Droplet Models

Trajectory of vaporizing particles from CFD





CFD Experiment of Air-Droplet Models



CFD Experiment of Air-Droplet Models

EE Number	Category	Critical EE	Corresponding D
EE<<1	Lazy particle	EE=0.01	D_{cr}=40µm
EE≈ 1	Vaporizing particle	0.01<EE<10	40µm <D<1500µm
EE>>1	Isothermal particle	EE=10	D_{cr}=1500µm

Note: The corresponding D is calculated with typical building parameters:

D_T=10m, H=3m, U=0.1m/s, ρ_p=1000kg/m^{3}, RH=40%, T=20°C

Conclusions

- Different particle and droplet CFD models provide different simulation results, in which size of particle and droplet is a critical justification factor.
- Stokes number and evaporation effectiveness number can be used as simple criteria to determine appropriate models.
- For typical indoor conditions, the rules of thumb are:
  - Particle

  - Droplet