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

(Annis 1991)

400 million/ft³ 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

\[ \mathbf{V} = 1 \text{m/s} \]

\[ v_{\text{particle}} = 1 \text{m/s} \]
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

\[ V = 1 \text{m/s} \]

\[ V_{\text{particle}} = ? \text{m/s} \]
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

\[ V = 1 \text{ m/s} \]

\[ V_{\text{particle}} = ? \text{ m/s} \]
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)**

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

- **Assumptions:**
  - Sphere particle or droplet
  - Particles size above 1 µm (so Brownian force excluded)
  - Particle density on the order of \(10^3\) kg/m³ 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; \(\rho_a=\)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 $f$

$$Re_r = \frac{\rho_a D |\vec{u} - \vec{v}|}{\mu_a}$$

$$f = \frac{C_D Re_r}{24}$$

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

$v =$ particle velocity; $u =$ air velocity; $\rho_a =$ air density; $\mu_a =$ air viscosity; $D =$ particle diameter; $\rho_p =$ 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

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

Clift and Gauvin (1970)

\[
f = 1 + 0.15 \operatorname{Re}_r^{0.687} + 0.0175 \times \left(1 + 4.25 \times 10^4 \operatorname{Re}_r^{-1.16}\right)^{-1}
\]
Analysis of Low Reynolds Particle Flow
(Re_r < 1) (Stokes Flow)

\[ \frac{dv}{dt} = \left( \frac{u - v}{\tau_v} \right) + g \]

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

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

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

\[ v_y = (u_y - \tau_v g) \left( 1 - e^{-t/\tau_v} \right) \]
Analysis of Low Reynolds Particle Flow (Re<1) (Stokes Flow)

If \( t = \infty \)

\[
\begin{align*}
\nu_x &= u_x \\
\nu_y &= (u_y - \tau_x g)
\end{align*}
\]

If \( t = \tau_v \)

\[
\begin{align*}
\nu_x &= 0.63 \cdot u_x \\
\nu_y &= 0.63 \cdot (u_y - \tau_v g)
\end{align*}
\]

So, the particle momentum response time \( \tau_v \) indicates how fast the particle can reach the air velocity and respond to the air velocity changes.
Definition: Stokes Number \( \text{St}_v = \frac{\tau_v}{\tau_F} \)

\( \tau_F \) is the characteristic time of a flow field that represents the shortest time for certain particle to be caught by obstructions.

Definition: \( \tau_F = \min\left(D_T/U, \sqrt{2H/g}\right) \)

<table>
<thead>
<tr>
<th>Stokes Number</th>
<th>Category</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{St}_v \ll 1 )</td>
<td>Lazy particle</td>
</tr>
<tr>
<td>( \text{St}_v \approx 1 )</td>
<td>Isothermal particle</td>
</tr>
<tr>
<td>( \text{St}_v \gg 1 )</td>
<td>Free dropping particle</td>
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</tbody>
</table>
Analysis of High Reynolds Particle Flow (Re_r > 1)

Re_r > 1 => f > 1 and f = F(Re_r)

\[ \frac{d \vec{v}}{dt} = \frac{(\vec{u} - \vec{v})}{\tau_v'} + \vec{g} \]

\[ \tau_v' = \frac{\rho_p D^2}{18 \mu_a} \left( \frac{1}{f} \right) \]

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.

![Graph showing the relationship between Re and \( \tau/(RoD^2/18\mu) \)]
Analysis of High Reynolds Particle Flow ($Re_r > 1$)

Stokes Number:

\[ St_v = \frac{\tau_{V=63\%U}}{\tau_F} \]

\[ \tau_F = \min\left(\frac{D_T}{U}, \sqrt{\frac{2H}{g}}\right) \]

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<td>$St_v &lt;&lt; 1$</td>
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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

![Graph showing the relationship between Stv and D (µm).](image-url)
# CFD Experiment of Air-Particle Models
(for both $Re_r > 1$ and $Re_r > 1$)

<table>
<thead>
<tr>
<th>Stokes Number</th>
<th>Category</th>
<th>Critical $St_v$</th>
<th>Corresponding $D$</th>
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</thead>
<tbody>
<tr>
<td>$St_v &lt; 1$</td>
<td>Lazy particle</td>
<td>$St_{v,cr} = 0.001$</td>
<td>$D_{cr} = 20 \mu m$</td>
</tr>
<tr>
<td>$St_v \approx 1$</td>
<td>Isothermal particle</td>
<td>$0.001 &lt; St_{v,cr} &lt; 10$</td>
<td>$20 \mu m &lt; D &lt; 1500 \mu m$</td>
</tr>
<tr>
<td>$St_v &gt;&gt; 1$</td>
<td>Free dropping particle</td>
<td>$St_{v,cr} = 10$</td>
<td>$D_{cr} = 1500 \mu m$</td>
</tr>
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Note: The corresponding $D$ is calculated with typical building parameters: $D_T = 10 m$, $H = 3 m$, $U = 0.1 m/s$, $\rho_p = 1000 kg/m^3$
Analysis of Droplet Flow in the Air

- **Droplet Momentum Equation**

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

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

\[
\frac{dm_p}{dt} = -\pi D_p \frac{K_v}{Cp_v} Nu \ln(1 + B_m)
\]

Or

\[
D_p \frac{dD_p}{dt} = -2 \frac{K_v}{Cp_v} \frac{Nu}{\rho_p} \ln(1 + B_m)
\]

- **Variables:**
  - \(m_p\): droplet mass
  - \(D_p\): droplet diameter
  - \(K_v\): thermal conductivity of droplet vapor
  - \(Cp_v\): specific heat capacity of droplet vapor
  - \(\rho_p\): particle density
  - \(Nu\): Nusselt number \(= 2(1+0.3Re^{0.5}Pr^{0.33})F\)
  - \(Re=\frac{D_p \rho_a |u-v|/\mu_a}\): Re=Reynolds number
  - \(Pr\): 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

\[ D_p \frac{dD_p}{dt} = -2 \frac{K_v}{C_p v} \frac{Nu}{\rho_p} \ln(1 + B_m) \approx \text{constant} \]

\[ D^2 = D^2_0 - \lambda t \]

\[ \lambda = 4 \frac{K_v}{C_p v} \frac{Nu}{\rho_p} \ln(1 + B_m) \]

\[ \tau_m = \frac{D^2_0}{\lambda} \quad \text{Evaporation Lifetime} \]
Analysis of Droplet Flow in the Air

- Definition: Evaporation Effectiveness Number
  \[ EE = \frac{\tau_m}{\tau_F} = \frac{D_0^2}{\lambda \tau_F} \]

- \( \tau_F \) is the characteristic time of a flow field that represents the shortest time for certain particle to be caught by obstructions.

- Definition: \( \tau_F = \min(D_T/U, \sqrt{2H/g}) \)

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<td>( \text{EE} \gg 1 )</td>
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CFD Experiment of Air-Droplet Models

Trajectory of vaporizing particles from CFD
CFD Experiment of Air-Droplet Models
## CFD Experiment of Air-Droplet Models

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<th>EE Number</th>
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<th>Critical EE</th>
<th>Corresponding D</th>
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<tr>
<td>EE&lt;&lt;1</td>
<td>Lazy particle</td>
<td>EE=0.01</td>
<td>D_{cr}=40µm</td>
</tr>
<tr>
<td>EE≈ 1</td>
<td>Vaporizing particle</td>
<td>0.01&lt;EE&lt;10</td>
<td>40µm &lt;D&lt;1500µm</td>
</tr>
<tr>
<td>EE&gt;&gt;1</td>
<td>Isothermal particle</td>
<td>EE=10</td>
<td>D_{cr}=1500µm</td>
</tr>
</tbody>
</table>

Note: The corresponding D is calculated with typical building parameters: 
D_T=10m, H=3m, U=0.1m/s, ρ_p=1000kg/m³, 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**
  - Lazy
  - 20 micron
  - Isothermal
  - 1500 micron
  - Free Dropping

  **Droplet**
  - Lazy
  - 40 micron
  - Vaporizing
  - 1500 micron
  - Free Dropping