Large Eddy Simulation of Human-induced Contaminant Transports

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Motivations

Contaminant Transports in Indoor Environments

Design of clean room

Design of ICU

Collective Protection Systems

• Design of ingress/egress units
• Optimization of airlock operations

http://www.abtech.net/hardwallcleanroom.html

http://www.engr.psu.edu/ae/iec/abe/control/isolation.asp

http://www.mschall.de/abc_schutz/colpro.html

Multizone Modeling or CFD ➔ Static environments with HVAC systems

Challenging issues

• Tracking of unexpected and sudden release of CB agents / infectious disease control
• Transient factors; ingress/egress, Human/door motions
Objectives

- Protections of indoor environments
  - Immune building / Collective Protection (ColPro) systems (Airlocks)
  - To protect building occupants from biochemical warfare agent attacks and from toxic materials released after industrial accidents
  - Transient factors: motion of personnel and doors, other forms of entry, vent system activity, etc.

- Simulation of time-dependent contaminant transports within room compartments, as caused by human motion and other factors
  - Development of methodology for complicated applications (networks of rooms, ventilation systems, opening /closing doors, complicated human motion, etc.) – Immersed Boundary Method
  - Use of detailed simulations to develop improved zonal models (e.g., CONTAM) for contaminant transport
  - Understanding of comprehensive contaminant transport mechanisms
Immersed Boundary Method

- Basic formulation – direct forcing

\[\rho \left( \frac{\partial u(x,t)}{\partial t} + u \cdot \nabla u \right) = \mu \Delta u(x,t) - \nabla p + f(x,t)\]

- Cell classifications
  - Heaviside function, G
  - Signed distance function, \(\Phi\)
    - Field points (G=0, \(\Phi>0\))
    - Band points (G=1, \(\Phi>0\))
    - Interior points (G=1, \(\Phi\leq0\))

Choi et al. (2007) Journal of Computational Physics
Immersed Boundary Method

- **Governing equations – direct forcing**
  - Continuity equation
    \[ R_{c}^{n+1,l} = (1 - G(\Phi^{n+1})) \left[ \frac{\partial (\rho u_j)^{n+1,l}}{\partial x_j} \right] + G(\Phi^{n+1}) \left[ \frac{p^{n+1,l} - p_B^{n+1,l}}{\beta^2 \Delta t} \right] = 0 \]
  - Momentum equations
    \[ R_i^{n+1,l} = (1 - G(\Phi^{n+1})) \left[ \rho \left( \frac{3}{2} u_i^{n+1,l} - 2u_i^n + \frac{1}{2} u_i^{n-1} \right) \right] \left[ \frac{\partial u_i}{\partial x_i} + \frac{\partial (\rho u_i u_j + \delta_{ij} p - \tau_{ij})^{n+1,l}}{\partial x_j} \right] \]
    \[ + G(\Phi^{n+1}) \rho \left[ \frac{u_i^{n+1,l} - u_{B,i}^{n+1,l}}{\Delta t} \right] = 0 \]
  - Contaminant transports (passive gaseous contaminants)
  - SGS eddy viscosity: Smagorinsky model
  - Preserving mass conservation of contaminant transports due to moving objects: tracer mass swept into or removed from a cell.
Immersed Boundary Method

Reconstruction (Interpolations near IB surfaces)

- Velocity interpolation
  - Power law for tangential velocity
  
  \[ u_{B,i}(n) = u_{T,i}(n) + u_{N,i}(n) + u_{s,i} \]

  \[ u_{T,i}(n) = \left\{ u_{T,i}(d_i) + \left(1 - \frac{n}{d_i}\right) \left[ k u_{T,i}(d_i) - d_i \frac{du_{T,i}}{dn} \right] (\frac{n}{d_i})^k \right\} \]

  \[ u_{N,i}(n) = \left\{ u_{N,i}(d_i) + \frac{1}{2} \left(1 - \left(\frac{n}{d_i}\right)^2\right) \left[ u_{N,i}(d_i) - d_i \frac{du_{N,i}}{dn} \right] (\frac{n}{d_i}) \right\} \]

- Pressure interpolation

  \[ p_B(n) = p_B(d_i) + B_n - \frac{1}{2} \left(\frac{dp}{dn}\right)_{n=d_i} + B \left(1 - \left(\frac{n}{d_i}\right)^2\right) d_i \]

- Interpolation point, \( d_i \)

  \[ d_i = \sum_{k} \omega_i(x_i - x_k) \cdot n, \]

  \( \omega \) : Weight based on merit function (inverse of projection distance)
Immersed Boundary Method

- **Surface Identifications & Signed Distance Function**
  - CAD-based surface rendering of immersed objects (Stereolithography (STL) file format)
  - Three vertices with outward-pointing normal vectors for each element
  - Distance calculation and surface identification
  - Calculation of distance from a given field point to the nearest surface point (O(M log N) algorithm) (Arya et al., 1988)
  - Calculation of signed distance function ($\phi$) using the dot product of the distance vector with outward angle weighted pseudo-normal vector (Bærentzen & Aanæs, 2005)
  - The zero iso-surface of the signed distance function is the body surface as represented on the field grid

Angle-weighted pseudo-normal vector
Realistic Human Walking Motion

- Human model + Ballistic walking motion (Mochon & McMahon, 1982)

Human surface (STL files)

Skeleton model for locomotion

Human rendering in the present computation.

\[
d_S = l^A (\sin \alpha_2^A - \sin \alpha_1^A) + l^B (\sin \alpha_2^B - \sin \alpha_1^B) + l^C (\sin \alpha_2^C - \sin \alpha_1^C)
\]
Contaminant Transports in Room Compartments

Problem specification

- Schematic diagram: three-compartment test rig

Problem parameters

- Walking velocity $V=1.25$ m/sec assumed in calculations
- Initial condition: $10$ ppm $SF_6$ in ‘dirty’ room
- Doors are opened and closed as man walks from dirty to clean rooms
- Vent located in center of vestibule (120 cubic feet / minute outflow)
- Vent activity for 60 s between walking events

Choi & Edwards (2011) Indoor Air
Contaminant Transports in Room Compartments

- Evolution of SF6 concentrations

![Diagram showing the evolution of SF6 concentrations in a room compartment at t=0.325. The color scale ranges from 1.0x10^{-36} to 2.0x10^{-4} with intermediate values.]
Contaminant Transports in Room Compartments

Time-dependent SF6 mass concentration for person walking event
Contaminant Transports in Room Compartments

- Five man walking/removal events
  - Time-dependent mass partitioning

![Graph showing mass transport dynamics over time](image)

<table>
<thead>
<tr>
<th>Man</th>
<th>Small vestibule</th>
<th>Large vestibule</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{cf}_{D\rightarrow V}$</td>
<td>$\text{cf}_{V\rightarrow C}$</td>
</tr>
<tr>
<td>1</td>
<td>42.7</td>
<td>11.3</td>
</tr>
<tr>
<td>2</td>
<td>25.1</td>
<td>28.4</td>
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<td>3</td>
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<td>7.28</td>
<td>32.4</td>
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<tr>
<td>5</td>
<td>2.95</td>
<td>31.8</td>
</tr>
<tr>
<td>Mean</td>
<td>29.8</td>
<td>23.3</td>
</tr>
</tbody>
</table>

- The net effect of increasing volume of the vestibule is to reduce the contaminant transport. (~20% reduction for 1.7 times larger vestibule)

- Vent activities (removal events) increase concentrations in vestibule (due to the entrainment from the gap beneath the first door).
- During the five-person walking events, mass transported into the clean room is ~4% of initial mass in the contaminated room.
Contaminant Transports in Room Compartments

- **Sensitivity analysis**
  - Categorized mass transports (dirty to clean room)
    - 30+ cases of single person walking events
    - Door type (sliding vs swinging)
    - Walking speed
    - Door opening rate
    - Walking pattern (stop/start vs continuous)
    - Initial pressure differential (0 to 20 pa)
  - Swinging door wake transport is the dominant effect
  - Net transport due to human wake motion alone is \( \sim 1.8 \text{ cf} \) and \( \sim 1.3 \text{ cf} \) for sliding and swinging door, respectively.
Contaminant Transports in Room Compartments

Multi-person walking event

Each man transports approximately the same amount of material into the clean room
Conclusions

General features

- Large-eddy simulation/Immersed boundary method for contaminant transport under human activities has been developed.

Contaminant transport in room compartments (airlock)

- Effect of vestibule size
  - Enlarging the vestibule size can reduce the contaminant transport.
    e.g., ~20% reduction for 1.7 times larger vestibule in the present configuration

- Effects of door type (sliding versus swinging), walking speed, and initial pressure differential on contaminant transport.
  - Swinging-door motion induces up to six times the amount of compartment-to-compartment transport than sliding door motion.
  - The human wake effect contributes about 67% of the total amount transported for sliding doors, while this value decreases to about 32% for swing-doors

- Effect of multi-person walking event
  - Each man transports approximately the same amount of material after a well-mixed state is reached.
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Thank you!