

Interlibrary Loans and Journal Article Requests

Notice Warning Concerning Copyright Restrictions:

The copyright law of the United States (Title 17, United States Code) governs the making of photocopies or other reproductions of copyrighted materials.

Under certain conditions specified in the law, libraries and archives are authorized to furnish a photocopy or other reproduction. One specified condition is that the photocopy or reproduction is not to be *“used for any purpose other than private study, scholarship, or research.”* If a user makes a request for, or later uses, a photocopy or reproduction for purposes in excess of “fair use,” that user may be liable for copyright infringement.

Upon receipt of this reproduction of the publication you have requested, you understand that the publication may be protected by copyright law. You also understand that you are expected to comply with copyright law and to limit your use to one for private study, scholarship, or research and not to systematically reproduce or in any way make available multiple copies of the publication.

The Stephen B. Thacker CDC Library reserves the right to refuse to accept a copying order if, in its judgment, fulfillment of the order would involve violation of copyright law.

Terms and Conditions for items sent by e-mail:

The contents of the attached document may be protected by copyright law. The [CDC copyright policy](#) outlines the responsibilities and guidance related to the reproduction of copyrighted materials at CDC. If the document is protected by copyright law, the following restrictions apply:

- You may print only one paper copy, from which you may not make further copies, except as maybe allowed by law.
- You may not make further electronic copies or convert the file into any other format.
- You may not cut and paste or otherwise alter the text.

FEDSM2003-45177

THE EFFECT OF TURBULENCE AND SCALAR TRANSPORT MODELS ON PREDICTION OF WORKER EXPOSURE TO AEROSOLS

Jun Li, Ismail B. Celik, Ibrahim Yavuz
Mechanical and Aerospace Engineering Department
West Virginia University, Morgantown, WV 26506

Steven E. Guffey
Industrial and Management Systems Engineering Department
West Virginia University, Morgantown, WV 26506

Aaron J. Bird
Centers for Disease Control and Prevention, National Institute for Occupational Safety and Health,
Health Effects Laboratory Division, 1095 Willowdale Road, Morgantown, WV 26505

ABSTRACT

The present study is concerned with the relative concentrations of contaminants in the breathing-zone (BZ) when toxic airborne contaminants are released within an arm-length in front of a worker, a common location that often leads to high exposures. Three-dimensional turbulent flow around a modeled human body in a wind tunnel has been simulated numerically and the results from various models are compared with each other. A model was built using a mesh generator to represent a real human body as closely as possible. Four different turbulence models, namely, standard $k-\epsilon$ turbulence model, RNG $k-\epsilon$ turbulence model, Reynolds Stress turbulence model (RSM) and Large Eddy Simulation (LES), were used to evaluate their effect on the predicted concentration levels used in assessing the exposure of the worker. Results from Eulerian scalar transport method and Lagrangian particle tracking method are also compared. Concentration levels are calculated at various sampling locations in the vicinity of the human face. It is found that the predicted concentration varies significantly from model to model: at the breathing zone the coefficient of variation for predicted concentration is 30%.

NOMENCLATURE

C	mean concentration
S	scalar source term
ρ	density
Re_p	particle Reynolds number
C_D	particle drag coefficient
D_p	diameter of the particle
ρ_p	density of the particle

u_p	velocity of the particle
σ_c	laminar Schmidt number
$\sigma_{c,t}$	turbulent Schmidt number
x_i	Cartesian coordinate in tensor notation
μ	fluid viscosity
t	time
T_{ke}	turbulent kinetic energy
K_{sgs}	subgrid scale turbulent kinetic energy

INTRODUCTION

Predicting and controlling human exposure to toxic airborne contaminants in the workplace is important. Occupational hygiene engineers, confronted with the design of ventilation systems to minimize human exposures to contaminants, need experimental data and modeling tools to assist in optimizing such controls.

Usually, wind tunnels are used to study experimentally the underlying mechanisms that control exposure levels. The factors which could affect the worker exposure in the wind tunnel (representing a work room) include: the contaminant generation rate and its position and momentum, the orientation of the worker, the facilities in the room, the inlet velocity, the turbulence intensity, the body temperature and the body shape. Of particular importance when comparing human subject results to those from mathematical modeling and mannequins are the effects of breathing and the motion of the worker.

Among all these factors turbulence levels and turbulence length scales associated with the turbulent eddies are probably one of the most important factors that will influence the dispersion of aerosol particulate. Hence, it is essential that turbulence models used are capable of accurately predicting the

major characteristics of the turbulent flows in the working environment. This very issue is the main topic of the present study. We performed simulations with four different models, namely, standard k- ϵ turbulence model, RNG k- ϵ turbulence model, Reynolds Stress turbulence model and Large Eddy Simulation (LES), and compared the predicted concentration levels at critical locations in the vicinity of the face of a simulated worker manikin. There is also an experimental component to this work which is currently underway (Guffey, 2003). The objective is to first perform predictions before the experiments are carried out so that the simulations are not biased, as is the case in much of the work presented in the literature. The results will be compared to experiments for assessment of relative performance of the commonly used turbulence models in the future.

We also use two different scalar transport models. In previous indoor airflow studies either Eulerian or Lagrangian methods were used to investigate the concentration field (Flynn and Sills, 2001; Kulmala et al., 1996; Hyun and Kleinstreuer, 2001). The comparison of the simulations with these two methods would be helpful in deciding which is better when analyzing human exposure to aerosols.

Our results from a previous experimental study with mannequins strongly support the supposition that lapel sampling does not well represent inhaled concentrations (Guffey et al., 2001). In this study, the concentrations at different locations are compared to determine the optimum sampling location and to determine errors from using samples taken at the lapel as the surrogate for inhaled concentrations. A concurrent experimental study with humans and mannequins also is examining whether sites on or near the face are better alternatives to sampling at the lapel.

COMPUTATIONAL DETAILS

In this study, a three-dimensional wind-tunnel simulation has been performed with the Fluent CFD software package (Fluent, Inc., Lebanon, NH). The geometrical configuration of the flow domain is shown in Figure 1, consisting of the wind tunnel (4.6m width \times 2.6m height \times 11m length), and a human body (1.78m height). The human body faces downstream of the flow. A moderately fine mesh was constructed with 136,302 nodes and 470,234 mixed cells. A cross cut from the 3-D mesh is shown in Figure 2. Much finer tetrahedral mesh was used around the human body and hexahedral elements were used in the other regions.

The governing equations solved are the well-known Reynolds Averaged Navier-Stokes equations (RANS) and the equation of continuity. In the RANS approach the turbulent stresses resulting from the time averaging of non-linear terms need to be calculated with an appropriate turbulence model, hence the use of turbulence models mentioned above.

In addition to the equation of motion, the energy equation was also solved. The buoyancy effects were included in the mathematical model.

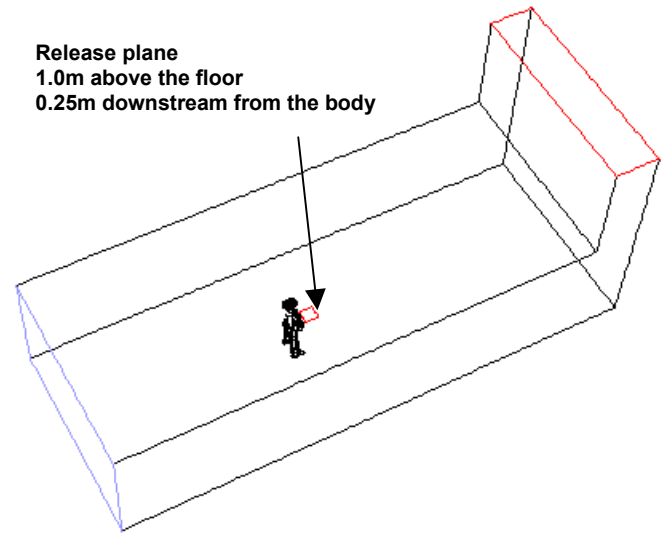


Figure 1 Schematic view of the wind tunnel model and location of release plane

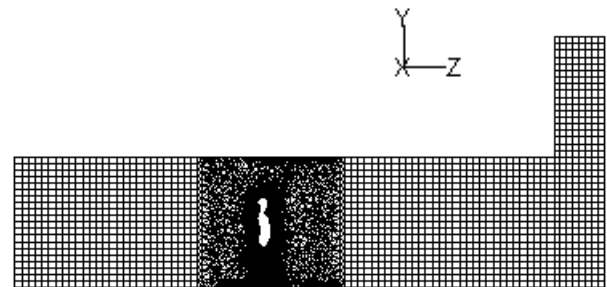


Figure 2 Example of a computational mesh used in the simulations

The governing equations employed for LES are obtained by filtering the time-dependent Navier-Stokes equations in physical space. The filtering process effectively filters out eddies whose scales are smaller than roughly the computational cell size. The resulting equations governing the dynamics of large eddies are very similar to the RANS equations, but in this case, the turbulent stresses are replaced by subgrid stresses. The Smagorinsky-Lilly subgrid-scale model (Lilly, 1966) is employed to solve the subgrid stresses in the present application. For values of the model constants and detailed information about these models, the reader is referred to the Fluent manual.

Constant velocity inlet and pressure outlet boundary conditions were used. The inlet velocity was taken as 0.3 m/s with a turbulence intensity of 0.3%. These values were rough estimates to the experimental conditions that would take place

in the future. However, we believe they are also representative of a usual working environment (Baldwin and Maynard, 1998). The characteristic length scale was chosen to be 0.01 m, which represented the turbulence generating grid size at the inlet of the tunnel. All of the solid walls in this investigation were at rest; therefore, both the mean and fluctuating velocities of the fluid at these boundaries were identically zero for the turbulent flow, as there was no slip and no mass-transport at the walls. Standard wall-function boundary condition was applied at the grid nodes nearest to the walls. Tracer gas was released from an inert surface, which was approximated by a 0.3m x 0.3m square and located 1.0m high from the floor and 0.25m downstream from the body.

The heat transfer boundary condition for the human body surface was taken as a convective heat flux of 16 W/m², which was based on a 2000-calorie diet and corresponds to a slight activity level of a standing person. Air was selected as the fluid medium and the tracer gas was nitrogen.

Eulerian Scalar Transport

If a species (e.g. nitrogen) is added to the system, the mean concentration of this species can be solved for using the following conservation equation:

$$\frac{\partial(\rho C)}{\partial t} + \frac{\partial}{\partial x_i} \left[\rho u_i C - \left(\frac{\mu}{\sigma_c} + \frac{\mu_t}{\sigma_{c,t}} \right) \frac{\partial C}{\partial x_i} \right] = S \quad (1)$$

Here σ_c is the laminar Schmidt number and $\sigma_{c,t}$ is the turbulent Schmidt number. In the present application the source term S is set to $0.0216 \times \rho$. The volume of this region is 0.00463 m^3 , such that the mass flow rate of the scalar is 0.0001 kg/s . The values of $\sigma_c = 0.32$ and $\sigma_{c,t} = 0.70$ (Lan and Viswanathan, 2001) are selected for the purpose of this study.

Lagrangian Particle Tracking

Particles are tracked according to a standard particle equation of motion:

$$\frac{du_p}{dt} = F_D(u - u_p) + g_x(\rho_p - \rho) / \rho_p + F_x \quad (2)$$

F_x term represents the other forces, in particular the diffusive force resulting from the fluctuating component of the fluid velocity. The drag function is given by

$$F_D = \frac{3\mu C_D \text{Re}_p}{4\rho_p D_p^2} \quad (3)$$

and the particle Reynolds number is

$$\text{Re}_p = \frac{\rho D_p |u_p - u|}{\mu} \quad (4)$$

The drag coefficient relation is

$$C_D = a_1 + \frac{a_2}{\text{Re}_p} + \frac{a_3}{\text{Re}_p^2} \quad (5)$$

In Eq.(5) a_1 , a_2 and a_3 are constants that apply for smooth spherical particles over several ranges of the particle Reynolds number Re_p given by Morsi and Alexander (1972). The particles are released from the plane shown in Figure 1. In order to conform to the Eulerian scalar transport method, the flow rate and diameter of the particles are set equal to 0.1 g/s and $1 \times 10^{-6} \text{ m}$, respectively.

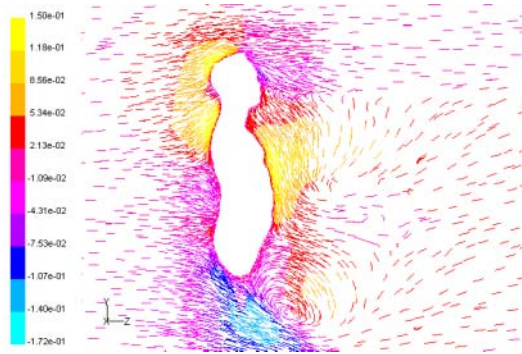
RESULTS AND DISCUSSION

Before comparing the results from different turbulence models, a grid sensitivity study was performed using approximately 30,000 nodes and 121,000 nodes. This has shown that the results from the finer grid could be considered more or less grid independent. Although a thorough grid convergence study is still necessary, in this study we shall be mainly concerned with trends.

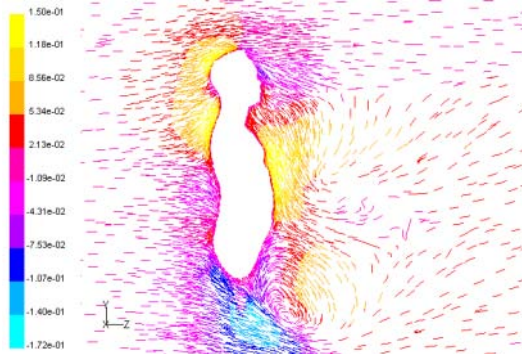
The streamlines colored by y-velocity magnitude on the center-plane are shown in Figure 3(a) for the case with standard k- ϵ turbulence model. As the plane slices the human-body in the center, the flow between the legs also can be seen in this figure, which will create a re-circulation region around the waist. The contaminants are usually trapped within such recirculation zones if turbulent diffusion is not dominant. It should be noted that if the worker wears an apron, the exposure he/she would receive could be quite different from the one observed in this study.

It can be seen from Figure 3 that the convective flow will bring the contaminant upward from the waist region. This flow is partly due to buoyancy as it is seen in Figure 4. This suggests that the heat flux from the human body could contribute to the worker exposure. Figure 3 shows that air flows along the forehead and separates from the body near the eye level. This means that such small issues as the hairstyle, the size and shape of the hat worn, and the angle of the forehead could be factors affecting the exposure levels.

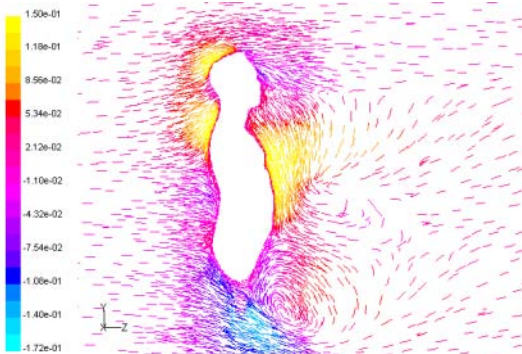
Figure 3 further shows us that the overall quantitative features of the flow patterns seen in the vicinity of the body are very similar for the RANS simulations irrespective of the turbulence model used. There are of course differences in the predicted turbulent kinetic energy profiles (see Fig. 5) when different turbulence models are used. The LES results (Fig. 3d), which were averaged over a three minute interval, do depict significantly different flow patterns compared to RANS results. This also translates into species concentration prediction as observed in Figure 8.



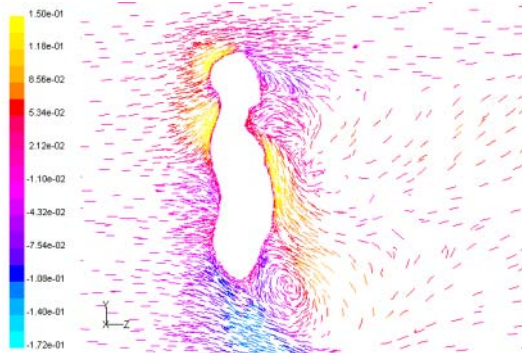
(a) Standard k-ε turbulence model



(b) RNG k-ε turbulence model

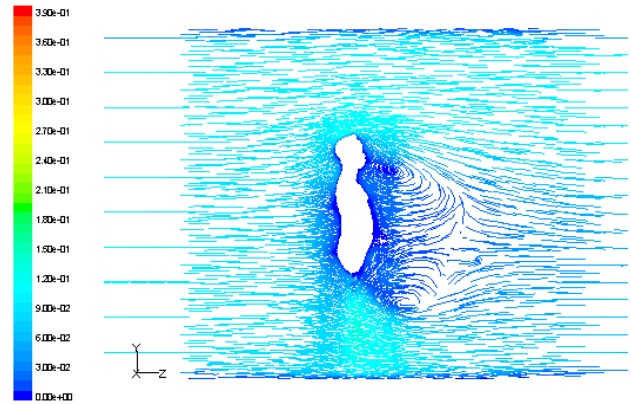


(c) RSM

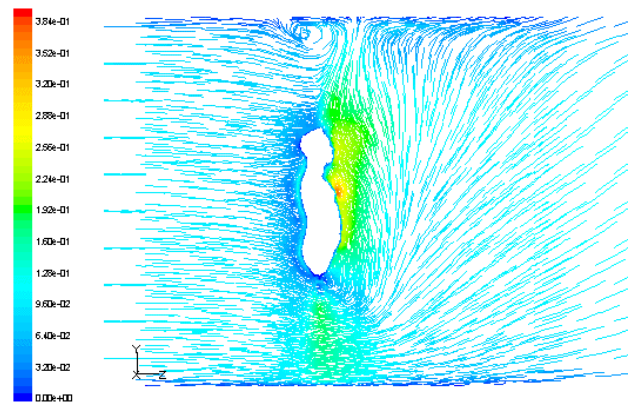


(d) LES (Averaged flow field)

Figure 3 Streamlines colored by y-velocity in the middle cross section plane with different turbulence models



(a) Heat loss rate of the body = 0 W/m²



(b) Heat loss rate of the body = 32 W/m²

Figure 4 Streamlines colored with velocity magnitude (This case is with Standard k-ε turbulence model and inlet velocity $v=0.1\text{m/s}$ which is different from the conditions used in other figures.)

The turbulent kinetic energy and the tracer gas concentration determined with the Eulerian method are depicted in Figure 5 and 6 for different turbulence models at different horizontal distances from the mouth along a vertical line in the middle plane. The standard k-ε turbulence model exhibited much higher turbulence kinetic energy levels than RNG turbulence model and RSM. This usually leads to a more diffusive concentration field. The turbulent kinetic energy profiles obtained from the RNG turbulence model and RSM are very similar. The subgrid turbulent kinetic energy, K_{sgs} , presented in Figure 5 indicates that most of the energetic large eddies are captured by the LES technique. Note that K_{sgs} represents the unresolved part of the turbulent kinetic energy by LES. This is apparent from the low levels of K_{sgs} compared to K obtained from RANS. As for computation time, RSM took approximately 50% more time than the RNG turbulence model which took a little bit more time than standard k-ε turbulence model. Because of its unsteady nature, the LES model required 200% more time than the RANS turbulence models. The contaminant concentration profiles shown at various locations

in Figure 6 indicate that except very near the body all models exhibit similar results. However, as seen in Figure 3d near the face of the body, LES results are significantly different than the other models.

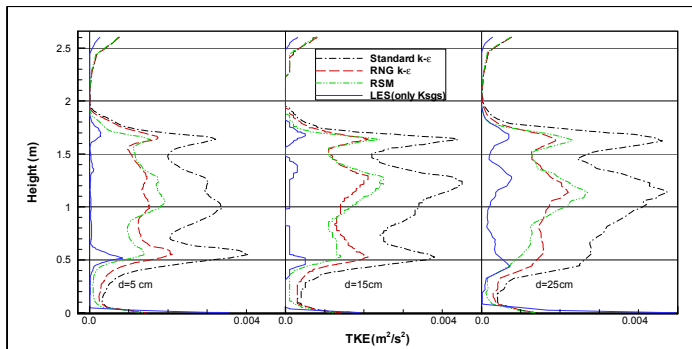


Figure 5 Tke/subgrid Tke at different horizontal distances from the mouth along a vertical line in the middle plane (Ksgs = Subgrid scale turbulent kinetic energy)

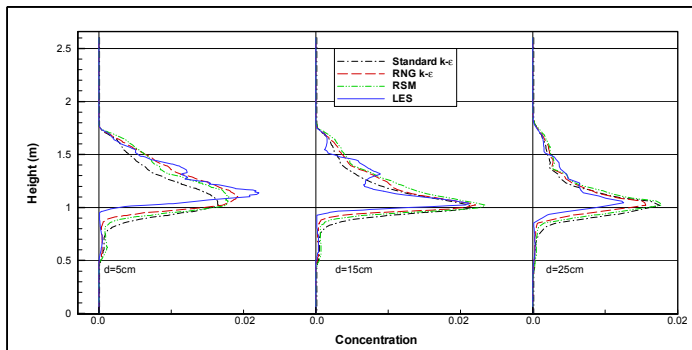


Figure 6 Scalar concentrations (kg/m³) at different horizontal distances from the mouth along a vertical line in the middle plane

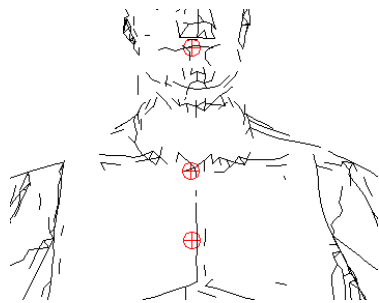


Figure 7 Sampling locations 1cm downstream of the body surface

It is believed that a useful measure of potential exposure to a worker may be obtained by sampling from three different locations within the breathing zone, as shown in Figure 7. The predicted concentration levels with the Eulerian scalar transport method and four turbulence models are compared at these locations (Figure 8). The concentration at the breathing zone is distinctively lower than the chest region, which suggest that the neck and the chest might not be good

surrogates for sampling worker exposure. On the other hand the conservative nature of the current sampling procedure near the chest would be viewed as a positive factor. The concentrations obtained from LES at the neck and the chest are much higher than those from RANS models. But the opposite trend can be observed at the nose region. This again demonstrates that LES exhibits less smeared concentration fields than RANS models.

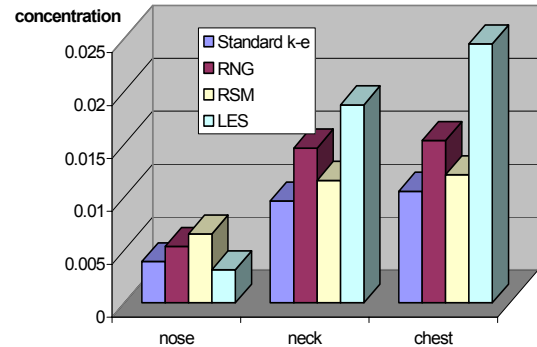
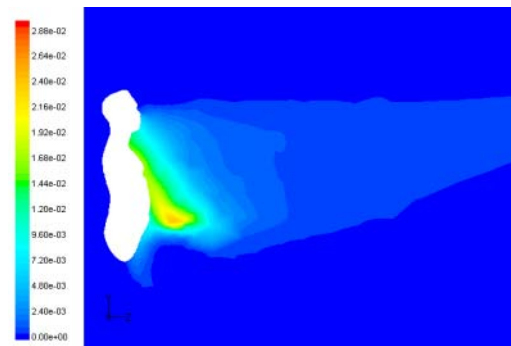
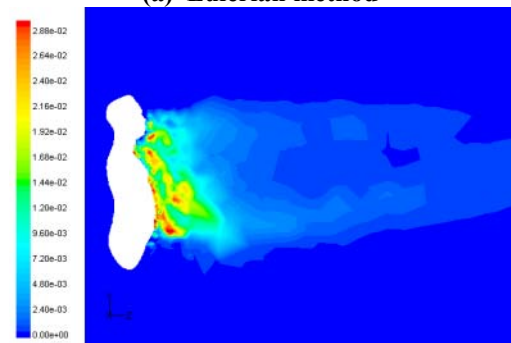


Figure 8 Concentration (kg/m³) levels at different sampling locations with different turbulence models; Eulerian scalar transport



(a) Eulerian method



(b) Lagrangian method

Figure 9 Concentration (kg/m³) field with different transport methods; RNG k-ε model

The results from Eulerian scalar transport method and Lagrangian particle tracking method are compared in Figure 9. The Lagrangian method shows much more chaotic distribution, which agrees with the simulation results done with a human-like body by Yavuz et al. (2003). It is clear that the Eulerian method exhibits a more diffusive pattern than the Lagrangian

method. It seems that the random fluid velocity fluctuations introduced into the equation of motion for particles via the F_x term in Eq.(2) recover some information lost in the averaged Eulerian equations by acting like a sub-grid scale model. The similarity of the concentration levels obtained from LES (Fig. 8) and those obtained from Lagrangian method used in conjunction with RNG k- ϵ model confirms the above assertion.

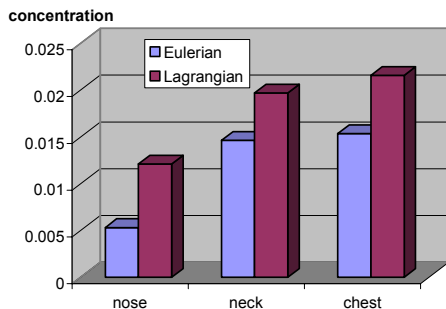


Figure 10 Concentration (kg/m³) levels at different locations with different transport methods; RNG k- ϵ model

Figure 10 compares the concentration levels for the Eulerian and Lagrangian methods. Both methods predict a lower concentration at the nose than other locations. But the levels at the neck and the chest predicted by Lagrangian is about 30% higher than the mean, and at the breathing zone it is about 80% higher.

CONCLUSIONS

The dispersion of contaminants in the vicinity of a simulated human working in a wind tunnel has been investigated using computational fluid dynamics technique. The flow in the wind tunnel represents a typical working environment, and the same wind tunnel will be used for a supplementary experimental work at West Virginia University. The objective was to assess the variations in predicted contaminant levels in the breathing zone of the worker when different turbulence models and scalar transport models are used.

The results from this show that significant differences in predicted concentration levels are observed when different models are utilized. The coefficient of variation for species concentrations predicted with four different turbulence models ranged between 30-40%. The difference between Lagrangian and Eulerian model predictions could be as high as 80%. The assessment of the relative performance of these models has to await the results of the experimental study. However, the present type of simulations can be used for trend analysis.

Under neutrally buoyant conditions, i.e. no convective component at the contaminant source, all models consistently predict higher concentrations at the neck and the chest level. The heat flux from the human body seems to have a significant

effect on the flow field. The Lagrangian scalar transport method produces much less varied concentration fields compared to those of the Eulerian method. A similar trend is observed when LES is used in conjunction with the Eulerian method. This indicates that RANS models when used with an appropriate Lagrangian transport method could be the best option for optimizing computational cost versus accuracy.

Given the uncertainty in modeling assumptions and the many other factors involved in predictions, we believe that a confidence interval for predicted concentration levels can be computed using the coefficient of variation for the results obtained from various turbulence models.

ACKNOWLEDGMENTS

This work has been performed under a U.S. National Institute for Occupational Safety and Health (NIOSH) project sponsored by Centers for Disease Control (CDC) under the grant R01 OH07587-01. We wish to acknowledge Paraform, Inc., Santa Clara, CA and Cyberware, Inc., Monterey, CA for providing the raw data used in the 3-D digitized human scan.

References

- S. E. Guffey, M. E. Flanagan, G. van Belle (2001) "Air Sampling at the Chest and Ear as Representative of the Breathing Zone." *AIHA Journal*. Vol. 62, No. 4, pp. 416-427.
- S. E. Guffey (2003) "Private Communication" Industrial and Management Systems Engineering Department, West Virginia University, Morgantown, WV 26506
- I. Yavuz, J. Li, I. B. Celik, and S. E. Guffey (2003) "CFD Simulation of Human Aerosol Exposure in a Wind Tunnel" accepted by the conference of British Occupational Hygiene Society Conference (April 8-10), Imperial College, London
- I. Kulmala, A. Saamanen and S. Enbom (1996) "The Effect of Contaminant Source Location on Worker Exposure in the Near-wake region." *Ann.Occup.Hyg.* Vol. 40, pp. 511-523.
- M. R. Flynn and E. D. Sills (2001) "Numerical Simulation of Human Exposure to Aerosols Generated During Compressed Air Spray-Painting in Cross-Flow Ventilated Booths", *ASME* Vol. 123, pp. 64-70.
- D. K. Lilly (1966) "On the Application of the Eddy Viscosity Concept in the Inertial Subrange of Turbulence" *NCAR Manuscript* 123.
- S. Hyun and C. Kleinstreuer (2001) "Numerical Simulation of Mixed Convection Heat and Mass Transfer in a Human Inhalation Test Chamber" *International Journal of Heat and Mass Transfer*. Vol. 44, pp. 2247-2260.
- S. A. Morsi and A. J. Alexander (1972) "An Investigation of Particle Trajectories in Two-phase Flow Systems" *Fluid Mech.* Vol. 55, Part2, pp. 193-208.
- N. S. Lan and S. Viswanathan (2001) "Numerical Simulation of Airflow Around a Variable Volume/Constant Face Velocity Fume Cupboard" *Am. Ind. Hyg. Assoc. J.* Vol. 62, pp. 303-312.
- P. E. J. Baldwin and A. D. Maynard (1998) "A Survey of Wind Speeds in Indoor Workplaces" *Ann. Occup. Hyg.*, Vol. 42, No. 5, pp. 303-313.