

Evaluating Uncertainties in Computational Fluid Dynamic Simulations of Human Exposure to Paint-Spray Aerosols

Flynn M R

Department of Environmental Sciences and Engineering, University of North Carolina, Chapel Hill, NC, USA

Introduction

Preliminary numerical simulations of human exposure to paint-spray aerosols demonstrate the ability of computational fluid dynamic (CFD) software to discriminate between two different orientations of spraying a flat plate in a cross-flow ventilated spray booth. (1) To conduct exposure-scenario simulations using CFD, a conceptual model of reality must be created that is compatible with the computer code. If this conceptual model is not a sufficient representation of reality with regard to the desired outcome, then no matter how accurate the simulation, the results will be of limited value. Conversely, good conceptual models will be inadequate, if there is insufficient numerical resolution. A balance between these two components is essential to achieve meaningful results given finite resources. This work examines some of the uncertainties involved in the conduct of such simulations with an eye toward developing efficient modeling approaches for optimizing control decisions based on exposure reduction.

Methods

Spray painting in cross-flow ventilated booths is a complex, time dependent, multi-phase problem. To construct tractable models of exposure, a hierarchy of approximations is invoked. The approach is first to construct a conceptual model capturing enough of the essential dynamics so as to provide a reasonable representation of the process with regard to exposure. This conceptual model is evaluated by comparing its predictions with real exposure data from field studies. The difference between the two defines one error that may or may not be important given the uncertainties in each. Second a numerical simulation is constructed based on the conceptual model. The difference between the numerical results and the conceptual model represents a second error, also subject to uncertainty. The relative magnitudes of these errors and uncertainties indicate limitations and where further refinements are needed.

A recent study(2) presents a conceptual model of exposure for compressed air spray painting applications. It is based on dimensional analysis and empirical data gathered in scale model wind tunnel studies, using a mannequin and non-volatile oil in lieu of paint. The model as summarized in equation (1), predicts a dimensionless breathing zone concentration as a function of an air momentum flux ratio and worker orientation.

$$\log_{10} \left(\frac{CHUD}{m_o} \right) = \alpha + \Delta \left(\frac{F_g}{F_m} \right)^\gamma \quad (1)$$

where α , Δ , and γ are constants dependent on geometry and orientation. C is the total mass concentration in the breathing zone; U is the average air velocity in the cross-flow spray booth (assumed uniform); H & D are the height and breadth of the worker; m_o is the overspray generation rate; F_g and F_m are the momentum flux of air from the gun, and through the projected area of the mannequin respectively; and Θ is the angle of orientation, 90° or 180° , (see Figure 1 below). Field studies(3) confirm its general applicability and provide an estimate of the uncertainty in using such an approach for real-world prediction. The model prediction was within one standard error of the measured mean exposure of 8 individuals based on a total of 56 discrete spraying tasks, when the work-piece was closely approximated as a flat plate. Given the variability of exposures, the conceptual model works well for the limited conditions it is designed to represent.

In a separate study, (1) numerical simulations were conducted to mimic the wind tunnel studies used to create the model defined above. Part of any numerical simulation is selecting the physical geometry to approximate the reality. Here a circular cylinder of height H and diameter D is used to represent the mannequin (worker). A square orifice on the surface of the cylinder of side length, s , is used to represent the spray nozzle as a jet of air. The face of this nozzle is at a distance, Z_p , from the plate. The velocities from the jet and into the wind tunnel were selected to match a specific momentum flux ratio for which experimental data were available.

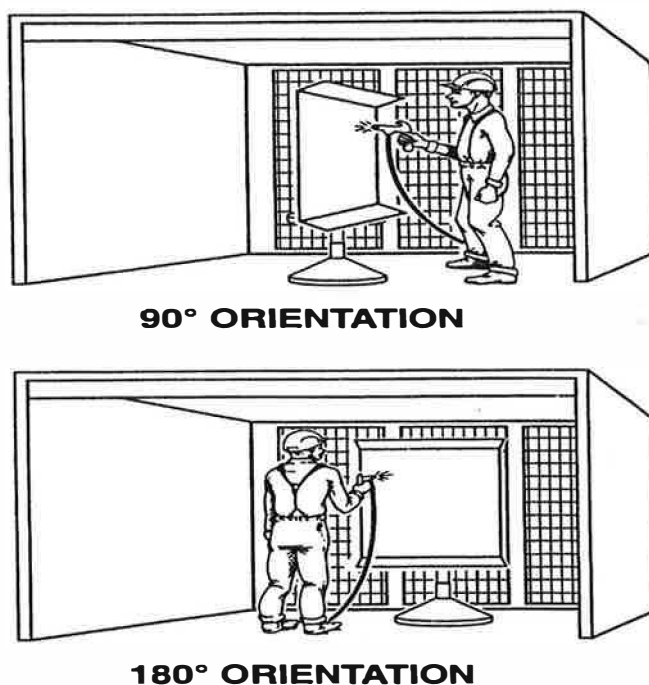


Figure 1. Orientations for spray painting in cross-flow booth

The approach was three-fold: (1) First, solve the three-dimensional, incompressible, steady-state, turbulent flow problem for the air velocity field. (2) Once the velocity field

is specified, aerosol particles are introduced at the center of the jet face and tracked through the flow field. (3) Finally the particle trajectories are converted into transfer efficiency predictions, breathing-zone mass concentrations and size distributions for comparison to the empirical data. The first two-steps are accomplished using the FIDAP finite element program. Step three is accomplished through development of an in-house algorithm to post-process FIDAP trajectory output.

Results

Table I presents a summary of the comparison between the simulation and empirical results. Numerical predictions of transfer efficiency converge to values of 0.77 and 0.78 for the 90° and 180° orientations respectively, while the experimental values were 0.94. The predicted dimensionless exposure for the 90o case is 1.08; while the comparable 180o prediction is 0 (undetected). The corresponding measured values were 0.14 and 0.0055. The numerical simulations correctly identify the orientation effect observed in the experiment, i.e., higher exposure in the 90o case; however, the quantitative agreement is poor. Numerically predicted transfer efficiency is about 80% of the measured value of 0.94; however this results in an overestimate for the mass generation rate by a factor of about 4.

Discussion and Conclusions

The observed differences between numerical simulation and experiment have many possible explanations but the error in transfer efficiency must be at the top of the list. The use of a 0.0254 m (1 in.) square orifice with a velocity of 35.56 m/s to simulate the actual spray-impaction process is clearly inadequate. The result is to dramatically overestimate the mass generation rate. The particles do not have sufficient momentum to impact, and thus become available for exposure. This suggests that reducing the size of the orifice, and increasing the velocities, while still maintaining the correct momentum flux ratio, should improve the prediction of transfer efficiency.

The comparability of the numerical predictions of aerosol concentration and size distribution with measured values is also problematic. Measured concentrations were gathered using open-face filters, while closed-face filters were used for the size distribution samples. The aspiration efficiency for the different orientations and samplers presents comparability questions with the numerical predictions.

Given the good agreement between field data and the empirical conceptual model, it seems clear that the main area for improvement is in the numerical simulation of the conceptual model i.e., higher resolution numerical simulations, with boundary conditions more closely matched to experimental conditions. In addition some method of accounting for particle sampling bias needs to be included – perhaps simulating the sampling process as well.

Acknowledgements

This work was supported by Grant Number R01/OH02858-06 from the U.S. National Institute of Occupational Safety and Health (NIOSH).

Table I. Summary of Simulated and Empirical Results

	Simulation Results		Empirical Results	
	A - 90°	B - 180°	A - 90°	B - 180°
Transfer Efficiency	0.77	0.78	0.94	0.94
Overspray m_o (g/s)	0.65	0.62	0.17	0.17
$CHUD/m_o$	1.08	0	0.14	0.0055
MMD (micrometers)	22.9	N/A	25.6	15.0
GSD	1.9	N/A	1.6	1.4

References

1. Flynn, M.R. and Sills, E.D. On the use of computational fluid dynamics in the prediction and control of exposure to airborne contaminants – an illustration using spray painting. *Ann. Occup. Hyg.* in press.
2. Flynn, M.R., Gatano, B., McKernan, J.L., Dunn, K., Blazicko, B.A., and Carlton, G.N. (1998). Modeling Breathing-Zone Concentrations of Airborne Contaminants Generated During Compressed Air Spray Painting, *Ann. Occup. Hyg.* 1999;42(1):67–76.
3. Carlton, G.N. and Flynn, M.R. (1997b), Field Evaluation of an Empirical-Conceptual Exposure Model, *Appl. Occup. Environ. Hyg* 12(8):555–561.