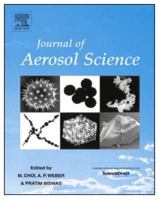
Journal of Aerosol Science 95 (2016) 54–66

Contents lists available at ScienceDirect

Journal of Aerosol Science

journal homepage: www.elsevier.com/locate/jaerosci



Three-dimensional computational fluid dynamics modeling of particle uptake by an occupational air sampler using manually-scaled and adaptive grids

Andrea C. Landázuri [a,b,*], A. Eduardo Sáez [a], T. Renée Anthony [c]

[a] *The University of Arizona, Department of Chemical and Environmental Engineering, 1133 E James E. Rogers Way, Tucson, AZ 85641, United States*
[b] *Universidad San Francisco de Quito USFQ, Colegio de Ciencias e Ingenierías "El Politécnico", Departamento de Ingeniería Química, Calle Diego de Robles y Vía Interoceánica, Cumbayá, Casilla Postal: 17-1200-841, Quito, Ecuador*
[c] *The University of Iowa, Department of Occupational and Environmental Health, 145 N. Riverside Drive, S300, Iowa City, IA 52242-5000, United States*

ARTICLE INFO

Article history:
Received 13 May 2015
Received in revised form
4 December 2015
Accepted 13 January 2016
Available online 22 January 2016

Keywords:
Computational fluid dynamics
Occupational sampler
k–ε model
Adaptive grid
Monotonic convergence
Turbulent flow

ABSTRACT

This work presents fluid flow and particle trajectory simulation studies to determine the aspiration efficiency of a horizontally oriented occupational air sampler using computational fluid dynamics (CFD). Grid adaption and manual scaling of the grids were applied to two sampler prototypes based on a 37-mm cassette. The standard k–ε model was used to simulate the turbulent air flow and a second order streamline-upwind discretization scheme was used to stabilize convective terms of the Navier–Stokes equations. Successively scaled grids for each configuration were created manually and by means of grid adaption using the velocity gradient in the main flow direction. Solutions were verified to assess iterative convergence, grid independence and monotonic convergence. Particle aspiration efficiencies determined for both prototype samplers were undistinguishable, indicating that the porous filter does not play a noticeable role in particle aspiration. Results conclude that grid adaption is a powerful tool that allows to refine specific regions that require lots of detail and therefore better resolve flow detail. It was verified that adaptive grids provided a higher number of locations with monotonic convergence than the manual grids and required the least computational effort.

1. Introduction

Occupational air samplers are used to assess human exposure to potentially toxic particulate matter due to inhalation. Typical samplers used for this purpose operate at flow rates between 2 and 4 L/min. However, research based on the prototypes presented in this work suggests that samplers could operate at suction flow rates as high as 10 L/min, which allows for sampling the same amount of air as with conventional samplers in a shorter period of time and, from another perspective, allows for reduction of the detection limit of sampled mass over the same period (Anthony & Flynn, 2006).

* Corresponding author at: Universidad San Francisco de Quito USFQ, Colegio de Ciencias e Ingenierías "El Politécnico", Departamento de Ingeniería Química, Calle Diego de Robles y Vía Interoceánica, Cumbayá, Casilla Postal: 17-1200-841, Quito, Ecuador.
E-mail address: alandazuri@usfq.edu.ec (A.C. Landázuri).

http://dx.doi.org/10.1016/j.jaerosci.2016.01.004
0021-8502/

CFD has been used as a tool to design sampling devices that monitor occupational exposure to aerosols that have the potential to cause respiratory system damage (Li, Lundgren & Rovel-Rixx, 2000). Direct experimental methods require the use of wind tunnels and are considerably more expensive than CFD simulations (Griffiths & Boysan, 1996), and modeling of occupational aerosol samplers using CFD generally has been based on two-dimensional simulations. The few three-dimensional studies usually lack geometric details due to memory or CPU limitations. Usual details that are left out include a realistic simulation of the sampler's inlet and the torso of the person on which the sampler is placed (Bird, 2005).

Convergence of the iterative methods and grid (or mesh) independence studies are of great importance prior to validation of the results obtained by CFD to ensure that comparison of the model with experimental data has genuine value (Tam et al., 2000, Richmond-Bryant, 2003). Iterative convergence and grid independence analyses are usually done following verification procedures described in previous works (Stern, Wilson, Coleman & Paterson, 2001, Roache, 1998) where three successively scaled grids are suggested for this purpose. However, it is important to consider that if the original grid is already very refined, the computational resources to generate and store the other two grids may become limited and simulations may take too long to converge to an appropriately low tolerance. On the other hand, if the original grid is too coarse, even two successively scaled grids may not be enough to obtain an accurate solution. Monotonic convergence is checked by calculation of the local mesh convergence ratio, defined by Roache (1998) as:

$$R_2 = \frac{\|e_{mid,fine}\|^2}{\|e_{coarse,mid}\|^2} \tag{1}$$

where

$$\|e\|^2 = \sqrt{\sum e_{j,k}^2} \tag{2}$$

and $e_{j,k}$ is the difference between the coarser (j) and finer (k) mesh level values for a given degree of freedom. Calculation of R_2 requires finding the numerical solution for three grid sizes (coarse, medium and fine). Mesh convergence is acceptable when local R_2 values are <1 for all degrees of freedom, which, for turbulent flows, include pressure (P), the three components of the time-averaged velocity (U_x, U_y, U_z), the turbulent kinetic energy (k) and the turbulent energy dissipation rate (ε).

In this work, both manual and adaptive grid scaling were used to verify the validity of the simulations. The grid quality of geometries such as the ones presented in this work required especial attention in order to avoid undesirable geometrical properties such as skewness, which can later influence in grid independence. All grids complied with the criterion of having a maximum skewness of less than 0.95 (Fluent, Inc, 2005).

Two 3-D facing-the wind, horizontally-oriented occupational samplers mounted on an elliptical torso, emulating the human body, and placed in a wind tunnel were considered. These samplers consist on a multi-orifice opening and were designed based on two-dimensional numerical studies. A multi-orifice inlet reduces wind effects and equalizes pressure variations inside the sampler, leading to uniformity in the deposition of particles on the filter. The sampler designs are based on the widely used three-piece 37-mm air sampling cassette and include a new sampling head that contains 1043 openings 254-μm in diameter. The prototypes presented in this work operate in conditions typical of indoor work environments at 293 K, 1 atm and a free-stream velocity of 0.4 m/s. One of the prototypes required an additional simulation parameter, which is the permeability of the filter. A more detailed discussion about the decision-making process for the proposed prototypes' design as well as the comparison of the model with respect to humanoid aspiration efficiency can be found elsewhere (Anthony, Landázuri, Van Dyke & Volckens, 2010).

The original grid used in the CFD calculations study contains triangular finite elements on each surface and tetrahedral elements to discretize the 3D domain. The final simulations were carried out using the standard k–ε model. This model shows good convergence and performs well for external flow problems around complex geometries (Fluent, Inc, 2005). Furthermore, based on a comparison of computation times, the standard k–ε model used relatively low memory requirements than the turbulent simulations using the RNG k–ε equations which were also tried, but its results have not been included in this work. The complete model runs with a pressure-based solver, along with the Green–Gauss cell-based discretization method for gradients and derivatives to generate iteratively the air flow field solution from the steady-state, incompressible, turbulent Navier–Stokes equations. Second order upwind schemes provide more accurate solutions than first order schemes, yet, depending on the nature of the problem, first order simulations may work adequately as well based on grid independence analysis (Fluent, Inc, 2005). The Green–Gauss node-based method is also known to provide more accurate solutions than the Green–Gauss cell-based method, but the former requires more computational time. Hence, since accuracy and less computational effort are crucial in this type of investigation, the final simulations were carried under second-order upwind schemes applied directly and using the Green–Gauss cell-based method. Once the fluid flow solution was evaluated, particle trajectory simulations were carried out to estimate the samplers' efficiency for particles with diameter in the range 6–100 μm.

Results from the simulations can be used to: (1) determine the effectiveness of the sampler to: (i) assess human exposure, (ii) improve sampler design and (iii) identify geometrical simplifications for grid generation depending on a specific interest; (2) emphasize the importance of grid convergence and grid independence assessment; and (3) recognize grid adaption as alternate tool to solve mixed flow regime problems.