Aerosol Generation Model for Cough Simulations

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The airborne transmission of disease is of great concern to the public health community because of the pandemic potential of newly emerging diseases like avian influenza. The possible spread of infectious disease by aerosols is of particular concern among health-care workers and emergency responders, who face a much greater risk of exposure to these hazards than does the general public. Influenza is believed to spread by dissemination and inhalation of aerosols of relatively small droplets that are produced by coughing and remain airborne for an extended time but the actual mechanisms of transmission are not well understood. For that reason a better understanding of the processes which lead to generation of aerosols is important. The goal of this study is to investigate the air-flow dynamics and the aerosol generation during coughing. A fairly simple model is developed for simulation of the flow inside the upper respiratory tract, focusing on the larynx and its vicinity, and to predict the number and size distribution of the aerosols generated during coughing. The aerosol generation and entrainment model (AGEM) is composed of droplet entrainment, generation and the break up models. The flow model solves for the velocity shear stress and pressure distribution, as well as the turbulent kinetic energy. These, in turn, are used as input parameters in AGEM to calculate the aerosol formations during a cough. The size distribution of the aerosol droplets after coughing is calculated and compared with the experimental results. The model is shown to be capable of calculating the size distribution of aerosols consistent with the experimental findings.

Theoretical Formulations. In the current pseudo two-dimensional study, a simplifying assumption has been made for the three-dimensional flow within the larynx to calculate the average velocity. The flow is governed by the one-dimensional continuity and momentum equations. For the numerical solution of the momentum equation the pressure-correction method is employed as proposed by MacCormack [1] and implemented by Tatli [2] and Celik et al. [3] and Ersahin [4].

Droplet Entrainment Model: The role of droplet entrainment model (DEM) is to calculate the total amount of mucus to be entrained into the system. The wall of the respiratory tract is assumed to be partially covered with mucus at a certain thickness depending on age, gender and health condition of the person. The thickness of the mucus and the fraction of the area covered with mucus are two of the unknowns at this stage of the study and need to be obtained from experiments. The Laursen formula for sediment discharge, which is used to calculate the total discharge in sediment transportation [5, 6], is modified to calculate the entrainment during the cough. The entrainment rate is taken to be proportional to diameter of the respiratory tract (D), turbulent kinetic energy (k), which represents the entrainment velocity, the wall shear stress (τ_w) and the critical shear stress (τ_{cr}). Rearranging these variables and introducing two model constants (C_ε and n) and a coefficient (ε) which defines the fraction of area covered with mucus to the inner surface area of the upper respiratory tract, the entrainment rate can be expressed as;

$$\frac{dE}{dt} = C_\varepsilon \varepsilon_A \frac{D^2}{2} \sqrt{k_{\max}} \left(\frac{\tau_w}{\tau_{cr}} - 1 \right)^n \qquad (1)$$

Selection of the model coefficients and the unknown physical properties, such as, the fraction of the area covered with mucus, is done in a way that the total amount of the entrainment matches the total amount of the aerosol generated during a cough measured experimentally. This is done only for one case; thereafter these values are retained.

Droplet Generation Model. Droplet generation model (DGM) takes the turbulence into consideration and determines the sizes of the drops formed. The maximum diameter of the droplets formed is a function of surface tension and the thickness of the mucus, the dissipation rate of the turbulent kinetic energy and turbulent length scale as given in [7];

$$D_{\max} = \min\left\{ C_B \left(\frac{\sigma}{\delta} \right)^{\frac{3}{5}} \varepsilon^{-\frac{2}{5}}, \ell_{tur} \right\} \qquad (2)$$

If the total amount of mucus entrained, E , and the maximum drop size, $D_{\max}$ are known, then the total number of droplets, n , can be calculated from the following relation.

$$n = \left\lceil \frac{E}{\frac{4}{3}\pi \left(\frac{D_{\max}}{2} \right)^3} \right\rceil \qquad (3)$$

Droplet Breakup Model. Although the droplet breakup can occur in different ways, it is common to assume a binary droplet breakup process and has been shown that it agrees well with the experimental measurements [8, 9]. During a binary breakup process the mother droplet divides into two daughter droplets. The sizes of the daughter droplets are less likely to be the same size. Therefore, the size of one of the daughter droplet is first calculated and the complementary daughter size is then obtained in such a way that the total mass is conserved. The sizes of the daughter droplets cannot be larger than the maximum drop size and smaller than the minimum drop size. Minimum drop size is a function of physical properties of the fluid making the droplet and the flow parameters and it is calculated from;

$$D_{\min} = \left(\frac{12\sigma}{\beta\rho D}\right)^{3/2} \varepsilon^{-1} \quad (4)$$

where ε is the turbulent dissipation rate of the air flow, σ ρ and are surface tension and density of the mucus fluid, respectively, D is the diameter of the mother droplet, and β is an empirical coefficient which is obtained experimentally to be 8.2 [10]. A random function is utilized in order to estimate the diameter of the first droplet. A pseudo-random number is generated within the range of [$D_{\min}$ - D_{mother}] and this number is assigned as the diameter of the first daughter droplet. Then the complementary daughter drop size is calculated.

Droplet Breakup Frequency. Droplet breakup frequency depends on a characteristic length and a characteristic velocity. Among other factors, the droplet diameter is selected as the characteristic length and the relative velocity is written as a function of the dissipation rate and the droplet diameter by following Kolmogorov's universal theory [11], which leads to the frequency time scale equation given by;

$$f_{breakup} = K_g \sqrt{\beta\left(\varepsilon d_0\right)^{2/3} - 12\frac{\sigma}{\rho d_0}} \Big/ d_0 \quad (5)$$

where K_g is found to be 0.25, experimentally, and β = 8.2 [12]. The value of is equal to the diameter of the mother droplet.

Turbulent Kinetic Energy Equation. Integration of the aerosol generation and the entrainment model into the one-dimensional flow field requires information about dissipation rate and turbulent kinetic energy from the main flow solver. This information is passed to the model through the solution of a one-dimensional integral turbulent kinetic energy equation. The solution of turbulent kinetic energy equation and passing the results to the model calculations is the most important interaction between the one-dimensional flow solver and the droplet models. The derivation of the integral turbulent kinetic energy equation can be found elsewhere [13, 14]. Here, the final form of the integral turbulent kinetic energy equation is given;

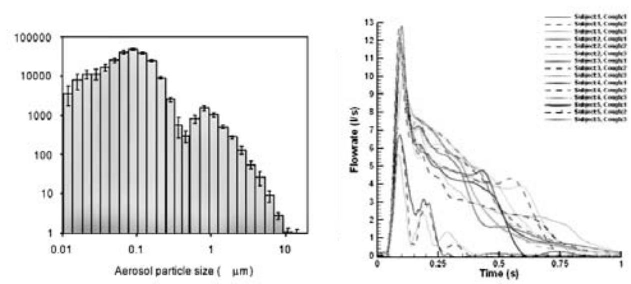
$$\frac{\partial}{\partial t}\left(\rho A \Delta x k\right) = \left(\rho u A k - \Gamma_k \rho A \frac{\partial k}{\partial x}\right)_w - \left(\rho u A k - \Gamma_k \rho A \frac{\partial k}{\partial x}\right)_e + G - D \quad (6)$$

where k represents the turbulent kinetic energy, ρ and u are density and average flow velocity, respectively, A is the cross-sectional area normal to the flow direction and Γ_k is the effective diffusivity. G and D denote turbulent kinetic energy generation and dissipation, respectively. Equations 1-6 constitute the mathematical model that is used to predict size and distribution produced from coughing.

Results and Discussion

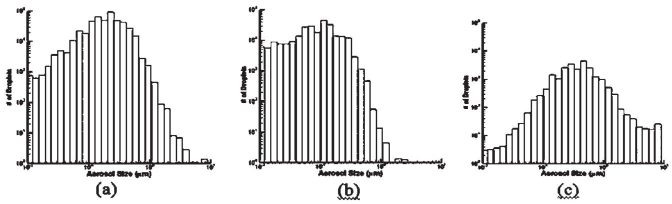
The model constants in the turbulent kinetic energy equation are tuned by comparison with a multi-dimensional, computational fluid dynamics model, namely FLUENT [15]. The tuning of the model coefficients in the aerosol generation and entrainment model are done in comparison to one set of experimental data available in hand [15]. The experimental data and the aerosol size distribution obtained by the proposed model is given in Figures 1 and 2a, respectively. It can be seen from the figures that, the model can produce similar results to the experimental measurements. The aerosol size distribution obtained by the model given in Figure 2a is the average of twelve different aerosol distributions for twelve different cough signals. In order to see the effects of different cough signals, aerosol size distribution for different cough signals are calculated. Since these cough signals were approximately equal to each other, it was expected to obtain similar results for each cough signal with some discrepancies. The random function, used in the binary droplet breakup mechanism, also has an effect on this similarity but not on the exact size distribution pattern. It is noted that, for the same coughing signal it is possible to obtain slightly different aerosol distribution every time the simulation is done. This reflects in a way the random nature of aerosol generation process. The effect of the physical properties of the mucus is also investigated and it is found that, the effect of the surface tension is the largest among the other physical properties. The density, viscosity and surface tension has been varied in the simulations and it has been noted that the effect of density and viscosity is much less than that of surface tension. In Figure 2, the aerosol size distribution is given for three different values of the surface tension. When the surface tension decreases, the number of aerosols increases since it is easier for them to break, and the size distribution shifts to left, with smaller aerosol size; when the surface tension increases, the opposite effect is observed. For more detailed study see [15].

Figure 1. a) Measured averaged aerosol size distribution during cough (The vertical axis is the concentration of aerosol); b) Coughing data obtained from NIOSH.



(a) (b)

Figure 2. (a) Averaged aerosol size distribution during a cough; Effect of surface tension on the distribution (b) 0.1σ; and (c) 10σ.



Conclusion

In this study a numerical model was developed in order to predict the aerosol size distribution during a cough. The model consists of sub-models, which make up the complete aerosol generation model that predicts the aerosol size distribution during a cough. This model is integrated into a one-dimensional flow solver, which simulates the flow in the upper respiratory tract and provides necessary information for the aerosol generation model through the solution of turbulent kinetic energy. Different coughing conditions have been simulated and an averaged aerosol size distribution was obtained. It was shown that the predicted aerosol size distribution is in good agreement with the experimental measurements. After tuning the model coefficients and predicting aerosol size distributions, which agrees with the experimental measurements, a parametrical study was carried out. The parametrical study has shown that the surface tension of the mucus affects the aerosol size distribution. As the surface tension increases, the size distribution shifts to the left producing larger aerosols. The present model shows that it is capable of predicting the aerosol size distribution during coughing, and it may be used in further studies to predict the physical properties of the mucus lining in the upper respiratory tract, and can be the included as a source term in predicting the aerosol dispersions in confined areas.

Acknowledgements

The support for this research by the National Institute for Occupational Safety and Health (NIOSH), Morgantown, WV is appreciated. The findings and conclusions in this report have not been formally disseminated by NIOSH and should not be construed to represent any agency determination or policy.

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Options for the Control of Influenza VI

June 17-23, 2007 • Toronto, Ontario, Canada

Editor

Jacqueline M Katz, PhD

INTERNATIONAL MEDICAL PRESS

Options for the Control of Influenza VI

Proceedings of the International Conference on Options for the Control of Influenza VI held in Toronto, Ontario, Canada
June 17-23, 2007

Editor

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Atlanta, Georgia, USA

International Medical Press

36 St Mary-at-Hill, London, EC3R 8DU
International Medical Press London, Atlanta

British Library in Publication Data

A catalogue record for this book is available from the British Library.

ISBN: 978-1-901-769-15-6

Printed and bound by Apex Book Manufacturing