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NUMERICAL PREDICTIONS OF TURBULENT FLOW AROUND A CUBE VIA THE $k-\epsilon$ MODEL*

by

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ABSTRACT

Turbulent air flows around structures are of importance in many engineering applications. Such flows can also have a significant impact on the thermal performance of the reactor vessel auxiliary cooling system of advanced liquid-metal reactor designs. The objective of the work presented in this paper was to evaluate the adequacy of the high-Reynolds-number form of the $k-\epsilon$ model in analyzing turbulent air flow around structures. An experiment of simulated atmospheric turbulent flow around a cube, performed by Castro and Robins, was analyzed with the computer code COMMIX and numerical predictions for pressure and velocity distributions were compared with experimental measurements. Considering the complexity of the problem and the approximations involved in the $k-\epsilon$ model, the overall agreement between numerical predictions and measurements of pressure coefficients and velocities was good. The largest discrepancies between predictions and measurements were in the pressure coefficient at the sections of the top and side cube surfaces very close to the upwind edges, and in the spanwise velocity distribution downstream from the cube.

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I. INTRODUCTION

Turbulent flows around structures are of importance in many engineering applications, like design of structures, dispersion of pollutants and contaminants, industrial ventilation, etc. Such flows can also have a significant impact on the thermal performance of the reactor vessel auxiliary cooling system (RVACS) of advanced liquid-metal reactor designs. The RVACS is one of the passive heat removal systems considered for decay heat removal in the current liquid-metal reactor (LMR) designs. It removes heat by natural circulation of air in the gap between the guard vessel and a baffle wall surrounding the guard vessel. The reactor heat is released to the atmosphere through a stack. The RVACS performance is a function of the pressure difference between airflow inlet and outlet, of the air density variation along the flow path, and of the pressure loss characteristics of this path. The pressure difference between inlet and outlet can be affected by wind velocity and direction. Wind may also lead to recirculation of heated exhaust air.

In Ref. 1, the computer code COMMIX² was used to analyze the effects of wind on the performance of the RVACS system of the PRISM advanced liquid metal reactor design. It was found that the RVACS performance can be significantly sensitive to wind speed and direction, but this sensitivity can be avoided by proper system design. The work of Ref. 1 presented the first opportunity to use COMMIX for this type of complicated turbulent flow. The objective of the work presented in this paper was to evaluate the adequacy of COMMIX, and more specifically of the k- ϵ model used in COMMIX, to analyze the turbulent air flow around buildings. For this purpose, an experiment performed by Castro and Robins³ was analyzed with COMMIX and code predictions for pressure and velocity distributions were compared with experimental measurements. This experiment has also been used by others to validate numerical predictions of turbulent flow around structures.^{4,5}

II. THE EXPERIMENT OF CASTRO AND ROBINS

Castro and Robins studied the turbulent flow around a cube placed on the floor of a wind tunnel. The wind tunnel system generated a 2 m thick boundary layer that was a 1/300 scale

simulation of a 600 m deep neutrally stable atmospheric boundary layer in an urban terrain. The wind mean velocity profile, u , in the boundary layer was well described by a power law of the form⁶

$$\frac{u}{u_0} = \left(\frac{z - d}{z_0} \right)^{0.25} \quad (1)$$

where z = vertical distance from the tunnel floor,
 d = zero plane displacement,
 z_0 = reference height,
 u_0 = velocity at z_0 .

This profile was also characterized by⁶

$$\frac{u^*}{u_{ref}} = 0.065, \quad \frac{z_r}{z_{ref}} = 0.0022, \quad \frac{d}{z_{ref}} = 0.01 \quad (2)$$

where u^* = friction velocity,
 z_{ref} = 2 m,
 u_{ref} = velocity at z_{ref} ,
 z_r = roughness length,
 d = zero plane displacement.

Terrain roughness was simulated by small wooden blocks placed on the tunnel floor as discussed in Ref. 6. The zero plane displacement, d , is a measure of the depth of the still air trapped among the roughness elements of the tunnel floor. In the absence of the cube, the velocity profile along the working section of the tunnel was nearly static (unchanged). The worst longitudinal mean velocity gradient was about 3% per 2 m. The experimental results of Ref. 3 show that the vertical profile of the mean velocity in the free stream has a significant effect on pressure and velocity distributions around a structure.

III. NUMERICAL MODEL

In the k-ε model, to simulate turbulence the Reynolds stress tensor $\overline{u_i u_j}$ of the averaged Navier-Stokes equations is approximated by

$$\overline{u_i u_j} = -\nu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad i = 1, 2, 3; \quad j = 1, 2, 3$$

where U_i = mean velocity in the i th direction,
 x_i = distance along the i th coordinate axis,
 u_i = fluctuation of the velocity component in the i th direction
 ν_t = kinematic turbulent viscosity

The turbulent viscosity ν_t is determined from

$$\nu_t = c_\mu k^2 / \epsilon$$

where c_μ is a constant and k and ϵ are the turbulent kinetic energy and the isotropic dissipation rate of k , respectively. The quantities k and ϵ are defined by

$$k = \frac{1}{2} \overline{u_i u_i}$$
$$\epsilon = \nu \overline{\left(\frac{\partial u_i}{\partial x_j} \right)^2}$$

and are determined from the partial differential equations of the k-ε model for k and ϵ .

The k-ε model used in COMMIX is based on the k-ε equations for high-Reynolds-number presented by Jones and Launder.⁷ These equations have been modified for use at low Reynolds numbers by incorporating correction terms which asymptotically lead to the high-Reynolds number equations as Re increases.²

In the model presented by Jones and Launder, the partial differential equations for k and ε were derived by manipulating the Navier-Stokes equations to obtain equations containing k and ε. To close these equations, the various unknown correlations contained in them were approximated in terms of calculable flow quantities, like k, ε and mean velocity gradients. The constants involved in these approximations were deduced as best estimates from experimental data.

The final equations of the k-ε model used in COMMIX-1AR/P to describe a turbulent flow are

$$\rho \frac{\partial k}{\partial t} + \rho U_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left\{ \left(\mu_t + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right\} + \mu_t \frac{\partial U_i}{\partial x_j} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \rho \epsilon$$

$$\rho \frac{\partial \epsilon}{\partial t} + \rho U_j \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left\{ \left(\mu_t + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right\} + \rho c_1 c_\mu k \frac{\partial U_i}{\partial x_j} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - c_2 \rho \frac{\epsilon^2}{k} f_\epsilon$$

$$\frac{\partial U_i}{\partial t} + \frac{\partial U_i U_j}{\partial x_j} = \frac{1}{\rho} \frac{\partial}{\partial x_j} \left((\mu_t + \mu_v) \frac{\partial U_i}{\partial x_j} \right) - \frac{1}{\rho} \frac{\partial p}{\partial x_i}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho U_i)}{\partial x_i} = 0$$

$$\mu_t = f_\mu c_\mu \rho k^2 / \epsilon$$

$$f_\epsilon = 1 - 0.3 \exp(-Re_t^2)$$

$$f_\mu = [1 - \exp(-Re_t/26.5)]^2$$

$$Re_t = \rho k^2 / (\mu_t \epsilon)$$

where p = mean pressure,

μ_t = dynamic laminar viscosity,

μ_t = dynamic turbulent viscosity,

and $c_\mu = 0.09$, $c_1 = 1.44$, $c_2 = 1.92$, $\sigma_k = 1.0$, $\sigma_\epsilon = 1.3$.

In COMMIX-1AR/P, for the numerical solution of the above differential equations the convection terms are discretized using the first order upwind scheme. First order differencing is also used for the diffusion terms. The discretized equations are solved iteratively. First the pressure equation, which results from a combination of the momentum equations and the continuity equation, is solved using the conjugate gradient technique. From the pressure solution and the momentum equations velocities are determined. Then, the k and ϵ equations are solved using successive-overrelaxation. This completes one outer iteration. The outer iterations are repeated until pressure, velocities, k and ϵ have converged for the current time step. For a steady state solution, only one outer iteration per time step is performed.

In Ref. 3, it is reported that at a distance of 8 h (h = cube height) downstream of the cube there was no discernible deviation of the mean velocity profile from the upstream boundary-layer profile, and even at 4 h the differences amounted to only a few percent. The main COMMIX calculations were based on a grid of 41 x 25 x 25 (xyz) and a computational space of 5 h upstream of the cube, 9 h downstream of the cube (total length in x direction = 15 h), 9.5 h in the y direction, and 6 h in the z direction (Fig. 1). Since the mean flow is symmetric in the y direction, only half of the cube was modeled. The mesh was finest next to the faces of the cube

and expanded in geometric progression away from the faces. Some variations in the grid structure and the size of the computational space were considered in a sensitivity analysis.

At the inlet of the computational space the distributions of the mean velocity (u), k and ϵ were specified. Free-slip was used at the boundary planes perpendicular to the y direction, as well as at the air-air interface in the z direction. For k and ϵ , at these boundaries the gradient normal to the boundary was set equal to zero. At the outlet, the pressure was set equal to the atmospheric pressure. Because the high-Reynolds-number form of the k - ϵ model is not valid very close to walls, for the computational cells adjacent to cube surfaces, boundary conditions were specified using a wall function formulation. For such a cell, the logarithmic law of the wall, for a smooth wall, was used to determine the wall shear stress from the velocity parallel to the wall at the center of the cell. The gradient of k normal to a wall was set equal to zero, and the value of ϵ at the center of a cell adjacent to the wall (ϵ_c) was determined from

$$\epsilon_c = \frac{c_\mu^{0.75} k_c^{1.5}}{K x_c} \quad (4)$$

where k_c = value of k at the center of the cell,
 K = von Karman constant = 0.42,
 x_c = the distance of the cell center from the wall.

Reference 3 gives the vertical profiles of mean longitudinal velocity, and turbulent intensity in an empty tunnel at the position of the cube, and for distances above the ground greater than about 0.5 h . There is no information provided for the inlet profile of ϵ . Consistent inlet profiles for the mean velocity, k and ϵ were determined by a series of calculations as follows. The cube was removed from the computational space and the x direction was extended to about 8 m. This length was limited by limitations of the current version of COMMIX on the total number of nodes in a given direction. The first calculation started with an inlet velocity profile given by Eq. (1), a k profile based on the turbulent intensity profile of Ref. 3, and a guess profile for ϵ . Then outlet velocity, k , and ϵ profiles determined from this calculation were used

as inlet profiles in the next calculation. The process was continued until these profiles did not change any further with distance in the flow direction.

These calculations were first performed by using on the ground the same boundary conditions as the ones discussed earlier for the cube surfaces, that is, the wall shear stress was determined from the logarithmic law of the wall for a smooth wall. It was found that the converged static velocity profile was drastically different than the initial inlet profile given by Eq. (1). This was not an acceptable result, because (a) in the experiment of Ref. 3 the boundary layer was nearly self-sustaining (the profile of mean velocity was nearly the same throughout the working section of the tunnel), and (b) as the experimental results of Ref. 3 show the wind velocity profile has a significant impact on pressure and velocity distributions around the cube. To avoid this problem, the velocity boundary condition on the ground was modified. The friction velocity was determined from

$$u^* = 0.065 u_{ref} \quad (5)$$

as measured in Ref. 6 for the conditions of the experiment of Castro and Robins. The combination of Eq. (1), power law velocity profile, and Eq. (5) with $z_{ref} = 2$ m gave

$$u^* = 0.0773 u/z^{0.25} \quad (6)$$

Equation (6) was used to determine the friction velocity, and consequently the wall shear stress, from the velocity at the center of a cell adjacent to the ground. With these modified boundary conditions, as Fig. 2 shows, a static velocity profile was calculated that was very close to the experimental profile of Ref. 3. This profile and the related k and ϵ profiles (Figs. 3 and 4) were used as inlet profiles in the COMMIX analysis.

Reference 3 gives the vertical distributions of $\bar{u}^2/u_{ref}^2$, $\bar{v}^2/u_{ref}^2$ and $\bar{w}^2/u_{ref}^2$ for the undisturbed flow at the position of the cube and for $z \geq 0.1$ m,

where u_{ref} = wind velocity at 2 m above the tunnel floor,

$\tilde{u}$, $\tilde{v}$, $\tilde{w}$ = velocity fluctuations in the x (flow direction), y, and z (vertical) directions.

For $u_{ref} = 14.973$ m, these distributions give $k = 3.4, 5.1$ and 4.6 at $z = 0.1$ m, 0.2 m and 1 m, respectively. As Fig. 3 shows, for the same range of z values the computed k varied from 0.6 to 2 and reached a peak value of 2.7 at $z = 0.04$ m. The computed k values were of the same order of magnitude as the measurements but consistently smaller.

IV. RESULTS

Reference 3 presents measurements of pressure on the surfaces of the cube and measurements of velocity above and downstream from the cube. The pressure measurements were made at Reynolds numbers (Re) greater than 10^5 and the velocity measurements at $Re > 3 \times 10^4$. No Reynolds number effects were discernible for $Re > 4 \times 10^3$. The Re number was based on the cube height and on the velocity at this height in the undisturbed flow. For the COMMIX analysis $Re = 10^5$ was used.

Figure 5 shows air flow patterns from the COMMIX analysis on two horizontal planes at $z/h = 0.074$ and $z/h = 0.609$, as well as on a vertical plane at $y/h = 0.065$. The flow on the horizontal planes shows separation on the cube side parallel to the axis of symmetry and is in agreement with the experiment and calculations presented in Refs. 4 and 7. COMMIX does not predict flow separation at the top of the cube, while separation close to the leading edge and reattachment further down was indicated by the experimental measurements and was predicted in Refs. 4 and 8, which also used the $k-\epsilon$ model for a similar analysis.

The pressure measurements of Ref. 3 were reported in the form of a pressure coefficient C_p defined by

$$C_p = (p_s - p_t) / 0.5 \rho u_t^2$$

where p_r = static pressure in the free stream above the boundary layer (2 m),
 p_s = static pressure on the surface of the cube at the point of interest,
 u_t = the velocity in the undisturbed flow at the cube height,
 ρ = air density.

Predicted pressure coefficients are shown in Fig. 6. These coefficients were computed at a distance of 0.0225 h from the cube surface while those of Castro and Robins were measured on the cube surface. The predicted values of C_p vary from -1.389 to 0.907 while the measurements of Ref. 3 range from -0.89 to 0.89. COMMIX overpredicted C_p on the lower section of the front face of the cube and underpredicted it on most of the other cube faces. Most severe are the underpredictions on the top and side surfaces of the cube very close to the upwind edges. The same experiment was analyzed with the k- ϵ model by Paterson et al⁴ and by Vasilic-Melling.⁵ The best agreement with the experimental measurements was achieved by Paterson et al. The COMMIX predictions lie between those of these two analyses. There are some differences in the k and ϵ boundary conditions used in this work and those used by Paterson et al. Their C_p predictions ranged from -1.31 to 0.92. Most notable is the use by Paterson et al of "a recirculation bubble promoter" to overcome the underprediction of the sizes of the recirculation zones formed at the upwind edges of the cube. This feature, which is not a part of the general k- ϵ methodology, is not used in COMMIX.

For a zero wind velocity, the driving pressure head of an RVACS system of an LMR like PRISM is about 100 Pa. For a reference velocity (at cube height) of 8.94 m/s (20 miles per hour), the maximum discrepancy in C_p between prediction and measurements of 1.389-0.89 corresponds to a pressure discrepancy of about 24 Pa. For the same velocity, the maximum discrepancies in C_p between predictions and measurements along the vertical lines C and D of Fig. 6 lead to pressure discrepancies of about 6 Pa.

Comparisons of predicted and measured vertical profiles of the longitudinal velocity above and downstream from the cube are presented in Fig. 7. The computed values correspond to $y/h = 0.065$, which is the closest computational point to the axis of symmetry in the flow direction. Fig. 7a shows values above the cube at $x/h = 0$ ($x = 0$, $y = 0$, $z = 0.2$ is the center of the top

cube surface). The location $x/h = 1$ (Fig. 7b) is 0.1 m downstream from the cube and most of the points below $z/h = 1$ are in a recirculation region. Finally, the location $x/h = 2.0$, Fig. 7c, is near the point of flow reattachment downstream from the cube. The agreement between predictions and measurements is good.

Transverse profiles of the longitudinal velocity at $z/h = 0.5$ and downstream from the cube are shown in Fig. 8. There is fair agreement between predictions and measurements, for example, at $y/h = 1$ the predicted velocities are about 19% higher than the measurements. This agreement is not as good as that of Ref. 4, but is better than that of Ref. 5.

As mentioned earlier, for the reference grid of $41 \times 25 \times 25$ COMMIX did not predict the small recirculation zone above the upwind section of the top of the cube. Such a zone was indicated by the experimental measurements, and was predicted in Refs. 4 and 8. The mesh size above the cube used in the COMMIX analysis was very comparable to that used in Refs. 4 and 8. To determine if a finer mesh would predict such a zone, the mesh interval in the z -direction just above the cube was halved and the computations were repeated with this grid of $41 \times 25 \times 26$. As Fig. 9 shows, with this grid a small recirculation zone above the upwind section of the top of the cube was predicted. However, this mesh refinement resulted in less accurate pressure coefficient predictions. For example, in Fig. 6 the maximum and minimum C_p values moved to 0.911 and -1.554 , respectively. A similar mesh refinement effect was observed in Ref. 4. The high-Reynolds-number form of the k - ϵ model is not valid very close to a wall. Moreover, the logarithmic law of the wall, which is used to define k - ϵ boundary conditions, is not valid in recirculating flow regions.⁹ One or both of these shortcomings may contribute to the loss of accuracy when a very fine mesh is used next to a wall.

Reference 4, which also used the first order upwind scheme, attributed the accuracy of its predictions to the use of the "ad hoc boundary condition called a recirculation bubble promoter. . . on the front edges of the cube. When this is replaced by wall function boundary conditions, there is a dramatic loss in accuracy in all variables." Reference 7, which also predicted the flow separation above the front section of the top of the cube, did not use the

"bubble promoter," but used a second order difference scheme for the momentum equations, instead of the first order upwind scheme used in COMMIX.

In Reference 4, Dirichlet boundary conditions were used on air-air interfaces, that is, the velocity was specified on these interfaces, instead of free-slip that was used in the COMMIX analysis. To determine the impact of the free-slip boundary conditions, computations were performed with a smaller computational space of 13 h x 4.5 h x 4 h (reference analysis used 15 h x 9.5 h x 6 h). The solution did not degrade significantly. For example, the maximum and minimum C_p values of Fig. 6 moved from 0.907 and -1.389 to 0.933 and -1.429, respectively. Therefore, the use of a free-slip boundary condition on air-air interfaces does not have a significant effect on the accuracy of the predictions.

Finally to determine the sensitivity of predictions to the grid structure, the analysis was repeated with a coarse grid of 21 x 13 x 13 by combining every two adjacent node-intervals of the reference grid into one. Comparisons of pressure coefficient and velocity predictions obtained with this grid and the reference grid are presented in Figs. 10, 11 and 12. These results show that a grid finer than the reference grid would not significantly improve prediction accuracy.

V. SUMMARY

The performance of an RVACS system can be significantly affected by wind speed and direction. The objective of this work was to evaluate the adequacy of COMMIX, and more specifically of the $k-\epsilon$ model used in COMMIX, to analyze the turbulent air flow around buildings. An experiment of simulated atmospheric turbulent flow around a cube, performed by Castro and Robins³, was analyzed with COMMIX and code predictions for pressure and velocity distributions were compared with experimental measurements. The flow around a cube immersed in a simulated turbulent atmospheric boundary layer is very complicated, and has all the major features of the flow around an RVACS stack. It involves high turbulence levels, flow separation and reattachment, and severe velocity and pressure gradients.

Considering the approximations involved in the k- ϵ model, the overall agreement between predictions and measurements of pressure coefficients and velocities is good. The largest discrepancies between predictions and measurements are in the pressure coefficient on the top and side cube surfaces very close to the upwind edges, and in the spanwise velocity distribution downstream from the cube.

Surface boundary conditions for k and ϵ are based on the logarithmic law of the wall, which is not valid in recirculating flow regions. This may contribute significantly to the discrepancies between predictions and measurements.

For the proper simulation of a static atmospheric boundary layer, the replacement of the logarithmic law of the wall for a smooth wall with the power law approximating the vertical distribution of the velocity in the simulated atmospheric boundary layer, and the use of a relationship for the friction velocity that was based on measurements were essential.

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Figure 1. Computational Grid

Figure 2. Inlet Velocity Profile

Figure 3. Inlet k Profile

Figure 4. Inlet ϵ Profile

Figure 5. Air Flow Patterns

Figure 6. Pressure Coefficients

Figure 7. Vertical Profiles of Longitudinal Velocity

Figure 8. Spanwise Profiles of Longitudinal Velocity

Figure 9. Air Flow Pattern for 41 x 25 x 26 Grid

Figure 10. Pressure Coefficient--Fine versus Coarse Mesh

Figure 11. Vertical Velocity Profiles--Fine versus Coarse Mesh

Figure 12. Spanwise Velocity Profiles--Fine versus Coarse Mesh

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