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# **An Implicit Finite-Difference Code for a Two-Equation Turbulence Model for Three-Dimensional Flows**

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Prepared for  
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AN IMPLICIT FINITE-DIFFERENCE CODE FOR A TWO-EQUATION TURBULENCE  
MODEL FOR THREE-DIMENSIONAL FLOWS

Upender K. Kaul\*

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SUMMARY

An implicit finite-difference code has been developed which solves the transport equations for the turbulence kinetic energy and its dissipation rate in generalized coordinates in three dimensions. The finite-difference equations are solved using the Beam-Warming algorithm. The kinetic energy-dissipation code, KEM, provides the closure; i.e., the turbulent viscosity for calculation of either compressible or incompressible flows. Turbulent internal flow over a backward-facing step has been calculated using the present code in conjunction with the Incompressible Navier-Stokes Code, INS3D. The results are in good agreement with experiments and two-dimensional computations of other researchers.

INTRODUCTION

There is a growing need for a two-equation turbulence model in generalized coordinates in three dimensions which can be used in conjunction with various flow codes that use the eddy viscosity calculated by an algebraic model of turbulence. Depending on the complexity of the geometry of application and that of the flow field, these codes should be able to choose between an algebraic and a two-equation turbulence model, the latter of which is described here.

Since the transport equations for the turbulence kinetic energy,  $k$ , and its dissipation rate,  $\epsilon$ , are not strongly coupled with the flow-field equations (e.g., see refs. 1 and 2), they are considered here as a candidate for the system of turbulence equations to be solved independently of the flow-field equations. These equations are solved implicitly as a two-by-two system in the present study, but are uncoupled from the flow-field equations. This paper gives the details of such a model run in conjunction with the incompressible Navier-Stokes code, INS3D (ref. 3), for a standard test problem (internal flow over a backward-facing step in a two-dimensional channel). The results are compared with results from experiments (ref. 4) and an earlier computation (ref. 1). Discussion of detailed computations

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(two dimensional) are given in reference 5. The model can be used with codes that solve either unsteady compressible or unsteady incompressible equations in generalized coordinates with viscous terms in all the three coordinate directions. A minor modification is needed to change from incompressible to compressible formulations as well as from fully viscous to thin layer formulations.

## GOVERNING EQUATIONS

The turbulence equations for  $k$  and  $\epsilon$  used here are cast in the conservation form. Using Einstein's index notation and the summation convention, transport equations for  $k$  and  $\epsilon$  can be written in Cartesian coordinates as the following two-by-two system, with  $k = (1/2)u_i u_i$  and  $\epsilon = (\mu/\rho)u_{i,j}u_{i,j}$ ;

$$\partial_t D + (F_i - F_{V_i})_{,i} = S \quad (1)$$

where the solution vector

$$D = \begin{bmatrix} \rho k \\ \rho \epsilon \end{bmatrix}$$

the flux vectors

$$F_i = \begin{bmatrix} \rho U_i k \\ \rho U_i \epsilon \end{bmatrix} \quad \text{and} \quad F_{V_i} = \frac{1}{Re_\infty} \begin{bmatrix} \mu k & k_{,i} \\ \mu \epsilon & \epsilon_{,i} \end{bmatrix}$$

and the source term

$$S = \frac{1}{Re_\infty} \begin{bmatrix} P - \rho \epsilon Re_\infty - 2\mu \frac{k}{d^2} \\ C_1 \frac{\epsilon}{k} P - C_2 f_2 \frac{\rho \epsilon^2}{k} Re_\infty - \frac{2\mu \epsilon}{d^2} f_3 \end{bmatrix}$$

The kinetic energy production term,  $P$ , is due to the mean shear and is given by  $-\rho u_i u_j U_{i,j}$  where  $U_i$  is the mean velocity and  $u_i$  is the fluctuating velocity. On application of the gradient diffusion hypothesis (Boussinesq, 1877), we can write the production term as

$$\left[ \mu_t (U_{i,j} + U_{j,i}) - \frac{2}{3} \rho k \delta_{ij} \right] U_{i,j}$$

where  $\delta_{ij}$  is the Kronecker delta and the turbulent viscosity  $\mu_t$  is given by Kolmogorov's hypothesis (ref. 6),  $\mu_t = C_\mu \rho k^{1/2} \ell$ . Since at high Reynolds numbers the dissipation rate,  $\epsilon$ , can be assumed to be proportional to  $k^{3/2}/\ell$ , we can write  $\mu_t = C_\mu \rho k^2/\epsilon$  where  $C_\mu$  is a constant.

Also,  $\mu_k = \mu + (\mu_t/\sigma_k)$  and  $\mu_\epsilon = \mu + (\mu_t/\sigma_\epsilon)$ , where  $\mu_t/\sigma_k$  and  $\mu_t/\sigma_\epsilon$  play the role of effective exchange or diffusion coefficients for  $k$  and  $\epsilon$ , respectively, and where  $\sigma_k$  and  $\sigma_\epsilon$  can be interpreted as turbulent Prandtl numbers for the  $k$  and  $\epsilon$  transport processes. Hence,  $\sigma_k$  and  $\sigma_\epsilon$  can be assumed to be close to unity in accordance with expectations; the turbulent viscosity is redefined as  $\mu_t = C_\mu f_\mu (\rho k^2/\epsilon) Re_\infty$ . The functions  $f_2$  and  $f_\mu$  above take into account the low Reynolds number dependence of the constants  $C_2$  and  $C_\mu$ , respectively (refs. 7 and 8), and they are defined as follows:

$$f_2 = [1.0 - \exp(-R_T^2)]^2$$

$$f_\mu = \exp \frac{-3.4}{(1 + R_T/50)^2}$$

The terms  $-2\mu k/d^2$  in the  $k$ -equation and  $(-2\mu\epsilon/d^2)f_3$  in the  $\epsilon$ -equation take into account the low Reynolds number effect near the walls and are due to reference 9. The function  $f_3$  is given by

$$f_3 = \exp \left( -C_3 \frac{\rho V_\tau d}{\mu} Re_\infty \right)$$

where  $V_\tau$  is the friction velocity and  $d$  is the normal distance to the wall. The values of the various "constants" are chosen as follows:

$$\sigma_\epsilon = 1.3$$

$$\sigma_k = 1.0$$

$$C_1 = 1.44$$

$$C_2 = 2.0$$

$$C_3 = 0.5$$

$$C_\mu = 0.09$$

The coefficient of viscosity  $\mu$  is normalized by  $\mu_\infty$ , velocities are normalized by  $U_\infty$ , distances by a characteristic length  $L$ , and the density  $\rho$  by  $\rho_\infty$ . This results in the reference Reynolds number definition as  $Re_\infty = \rho_\infty U_\infty L / \mu_\infty$ , normalization of  $k$  by  $U_\infty^2$ , and that of  $\epsilon$  by  $U_\infty^3/L$ .

The transport equation for turbulence kinetic energy is obtained by taking the moment of the instantaneous form of the Navier-Stokes equations, adding and then averaging them (the square root of the turbulence kinetic energy represents a velocity scale of the turbulent motion). The assumption of the gradient-diffusion model for  $k$  is introduced, i.e., the viscous diffusion of flux of  $k$  is proportional to the gradient of  $k$ . The  $k$  equation takes into account the history and transport effects of turbulence which the mixing length hypothesis cannot account for, since it is based on the assumption of local equilibrium everywhere in the flow field. The local equilibrium assumption is that the turbulence produced at a given point in the flow field is dissipated at the same rate as it is produced, thereby exerting no influence on the flow field at other points at a later time. Also from the mixing length hypothesis, the turbulent viscosity vanishes at those points in the flow field where the velocity gradients vanish, which is not true in general.

Some researchers (e.g., ref. 10) have derived a transport equation for the length scale of the turbulent motion represented by  $\lambda$ , and it has been used with the  $k$  equation in modeling a turbulent flow field (e.g., refs. 11 and 12). The turbulence length scale equation also accounts for the history and transport effects of turbulence. However, the specification of an appropriate length scale in the  $k$ - $\lambda$  system at the boundaries is a difficult task. The transport equation for the turbulence kinetic energy dissipation rate is derived based on physical considerations, and the number of the constants in the  $k$ - $\epsilon$  model is one less than in the  $k$ - $\lambda$  model or any other two-equation model. The wall boundary conditions for the dissipation rate  $\epsilon$  are relatively easy to prescribe. Although an exact equation for the dissipation rate,  $\epsilon$ , can be derived from the instantaneous form of the Navier-Stokes equations (ref. 13), the transport equation for  $\epsilon$  used here is based on heuristic grounds (ref. 14) since the exact equation requires drastic model assumptions that yield an  $\epsilon$  equation with a highly empirical character.

The equations for  $k$  and  $\epsilon$  given here are applicable for both the high and low turbulent Reynolds number,  $R_T = (\rho k^2 / \mu \epsilon) Re_\infty$ . Near the wall, the high-Reynolds number form of the  $k$ - $\epsilon$  system is modified as follows: (1) the viscous diffusion of  $k$  and  $\epsilon$  is included in the governing equations, and (2) the constants  $C_2$  and  $C_\mu$  are allowed to be functions of the turbulent Reynolds number,  $R_T$ , and appropriate terms are added to the high-Reynolds number form of the  $k$  and  $\epsilon$  equations (refs. 7-9). Since the total dissipation rate is not zero at the wall and the isotropic dissipation there vanishes, a term for the dissipation at the wall is chosen which corresponds to the nonisotropic part of the energy dissipation.

Accordingly, the term  $-2\mu(k/d^2)$  is added to the right-hand side of the  $k$  equation (ref. 9). With both the high- and low-Reynolds number forms thus built into the  $k$ - $\epsilon$  system, the governing equations can be solved subject to the boundary conditions applied either at the wall, or away from the wall through the use of wall functions (ref. 15).

Using the generalized coordinate transformation,

$$\tau \equiv t$$

$$x_j \equiv x_j(x_i, t)$$

where  $x_j = (\xi, \eta, \zeta)$  and  $x_i = (x, y, z)$  the  $k$ - $\epsilon$  system transforms to

$$\partial_\tau \bar{D} + \partial_{x_i} (\bar{F}_i - \bar{F}_{v_i}) = \frac{1}{J} S \quad (2)$$

where the solution vector,

$$\bar{D} = \frac{1}{J} \begin{bmatrix} \rho k \\ \rho \epsilon \end{bmatrix}$$

and the flux vectors,

$$\bar{F}_i = \frac{1}{J} \begin{bmatrix} \rho k Q_i \\ \rho \epsilon Q_i \end{bmatrix} \quad \text{and} \quad \bar{F}_{v_i} = \frac{1}{J} \frac{1}{Re_\infty} \begin{bmatrix} \mu_k & \nabla x_i \cdot \nabla x_i & \partial x_i k \\ \mu_\epsilon & \nabla x_i \cdot \nabla x_i & \partial x_i \epsilon \end{bmatrix}$$

The Jacobian,  $J$  is given by

$$J = \frac{\partial x_i}{\partial x_j}$$

and the contravariant velocities are given by

$$Q_i = \partial_t x_i + U_j \partial_{x_j} x_i$$

#### BOUNDARY CONDITIONS

There are two ways to incorporate the boundary conditions on  $k$  and  $\epsilon$  at the walls in the  $k$ - $\epsilon$  system. In the first case, Dirichlet wall boundary conditions

are chosen so that  $k = 0$  and  $\epsilon = 0$  at the walls (the nonisotropic part of the dissipation rate at the wall is included in the  $k$  equation and a similar "wall" dissipation term is added to the  $\epsilon$  equation that permits setting  $\epsilon$  equal to zero at the walls (ref. 9)); in the second case, the wall function approach is adopted which precludes having to integrate right down to the walls and thereby the stiffness problem associated with the first approach is avoided. In the present code, both options are available. Dirichlet inflow conditions and Neumann outflow and far-field conditions are used to complete the necessary boundary condition procedure.

A wall function approach (ref. 15) is used to connect the outer region to the viscous sublayer. The assumption here is that the resultant tangential velocity at a point  $P$ , which is located near the wall outside the viscous sublayer, follows the logarithmic law of the wall, and that the turbulence is in local equilibrium at such a point, i.e., that the rate of production of the turbulence kinetic energy equals the rate at which it is dissipated. Then, at such a point,  $P$ , we have

$$\frac{V_P}{V_\tau} = \frac{1}{\kappa} \ln \left[ E \frac{V_\tau d_P}{\mu} Re_\infty \right]$$

where  $E$  is a parameter which accounts for surface roughness or friction, or phenomena such as pressure gradient or mass injection through the walls, where  $\kappa$  is the von Karman constant ( $= 0.42$ ),  $V_P$  is the resultant tangential velocity at  $P$ ,  $V_\tau$  is the resultant friction velocity and is equal to  $\sqrt{\tau_w/\rho}$ , and where  $d_P$  is the normal distance between  $P$  and the wall. The kinetic energy and the dissipation rate at  $P$  are then given by

$$k_P = \frac{V_\tau^2}{\sqrt{C_\mu}} \quad \text{and} \quad \epsilon_P = \frac{V_\tau^3}{\kappa d_P}$$

#### NUMERICAL SCHEME

The numerical scheme used to solve the  $k$ - $\epsilon$  system, equation (2), is the implicit, noniterative approximate factorization algorithm of Beam and Warming (ref. 16). Before finite differencing the equations, the flux vector  $F_{V_i}$  in equation (1) is redefined as

$$F_{V_i} = \frac{1}{\rho Re_\infty} \begin{bmatrix} \mu_k(\rho k), i \\ \mu_\epsilon(\rho \epsilon), i \end{bmatrix} - \frac{1}{\rho^2 Re_\infty} \begin{bmatrix} \rho k \mu_k & \rho, i \\ \rho \epsilon \mu_\epsilon & \rho, i \end{bmatrix}$$



so that the second term is lumped explicitly with the source term, S. Writing the finite-difference expression for equation (2), we have

$$\frac{D^{n+1}}{J^{n+1}} + \Delta\tau \left[ \delta_{\chi_i} \left( \bar{F}_i - \bar{F}_{v_i} \right)^{n+1} \right] = \frac{D^n}{J^n} + \frac{\Delta\tau}{J^n} S \quad (3)$$

where the time-differencing is first-order (Euler) implicit, and the spatial derivatives are approximated by the central-differencing operator  $\delta_{\chi_i}$ .

Linearizing the flux vector  $\bar{F}_i$  locally in time, equation (3) can be written as

$$\begin{aligned} & \left\{ I + J^{n+1} \Delta\tau \left[ \delta_{\chi_i} \left( \bar{M}_i^n - \frac{\alpha}{\rho} \delta_{\chi_i} \right) \right] \right\} (D^{n+1} - D^n) \\ & = \frac{J^{n+1}}{J^n} (D^n + \Delta\tau S) - ID^n - \Delta\tau J^{n+1} \left\{ \delta_{\chi_i} \left[ \left( \bar{F}_i^n - \frac{\alpha}{\rho} \delta_{\chi_i} D^n \right) + \frac{\alpha}{\rho^2} \left( \delta_{\chi_i \rho} \right) D^n \right] \right\} \quad (4) \end{aligned}$$

where the Jacobian matrix of the flux vector  $\bar{F}_i$  is given by

$$\bar{M}_i \equiv (\bar{A}, \bar{B}, \bar{C}) = \partial_{\bar{D}} \bar{F}_i^n = \frac{1}{J^n} \begin{bmatrix} Q_i & 0 \\ 0 & Q_i \end{bmatrix}$$

$$\alpha = \frac{\Gamma}{J^{n+1} Re_\infty} \nabla \chi_i \cdot \nabla \chi_i$$

with

$$\Gamma = \begin{bmatrix} \mu_k & 0 \\ 0 & \mu_\epsilon \end{bmatrix}$$

The right-hand side of equation (4) is calculated explicitly, and the left-hand side can be factored approximately. Therefore, we have

$$\left[ I + \frac{\Delta\tau}{2} J^{n+1} \delta_{\xi} \left( \bar{A}^n - \frac{\alpha}{\rho} \delta_{\xi} \right) + \epsilon_i \nabla_{\xi} \Delta_{\xi} \right] \left[ I + \frac{\Delta\tau}{2} J^{n+1} \delta_{\eta} \left( \bar{B}^n - \frac{\alpha}{\rho} \delta_{\eta} \right) + \epsilon_i \nabla_{\eta} \Delta_{\eta} \right] \\ \times \left[ I + \frac{\Delta\tau}{2} J^{n+1} \delta_{\zeta} \left( \bar{C}^n - \frac{\alpha}{\rho} \delta_{\zeta} \right) + \epsilon_i \nabla_{\zeta} \Delta_{\zeta} \right] (D^{n+1} - D^n) = \text{RHS} - \epsilon_e [(\nabla_{\chi_i} \Delta_{\chi_i})^2] D^n$$

where  $\nabla$  and  $\Delta$  are first-order forward- and backward-difference operators, RHS is the right-hand side of equation (4),  $\epsilon_i$  is the implicit second-order smoothing parameter, and  $\epsilon_e$  is the explicit fourth-order smoothing parameter. The smoothing terms are added to damp the high frequency oscillations in the solution which arise out of the central-difference approximation of the spatial derivatives.

### CODE VALIDATION RESULTS

The k- $\epsilon$  turbulence model code, KEM, which is developed here, is tested and validated by computing the flow over a backward-facing step, by comparing the predictions with experiments (ref. 4), and by using earlier computations (ref. 1). For detailed simulations, the reader is referred to reference 5.

Since the present computations were carried out with the primary purpose of validating the KEM code, only preliminary results showing a comparison of the present predictions with experimental data and with an earlier computation are given here.

Figure 1 shows the plot of stream function contours over the back-step. The length of the separation bubble is somewhat underpredicted. A reasonable comparison is made of mean velocity at a location of 5.2 step heights downstream of the step as it is plotted against the cross flow coordinate in figure 2. Figure 3 shows the turbulence kinetic energy variation along the crossflow coordinate at 7.7 step heights downstream of the step. Finally, figure 4 shows the pressure distribution along the streamwise direction on the step side wall. Again, the comparison is reasonable.

### CONCLUSIONS

The KEM code offers the capability of predicting the compressible or incompressible three-dimensional turbulent flows around arbitrary geometries in external and internal flow situations in conjunction with any flow solver. The code is robust and easy to use. The use of the code necessitates allocation of additional computer memory for the two scalar variables, the turbulence kinetic energy and the dissipation rate. It predicts complex turbulent flows with large separated and secondary flow regions satisfactorily. For flows with strong pressure gradients and curvature

effects, the turbulence model employed here may need appropriate corrections to yield more accurate results.

#### ADDENDUM

A more realistic alternative boundary condition formulation has been used yielding results in better agreement with experimental data. This formulation is based on the near wall behavior of turbulence<sup>17</sup> and yields the following boundary condition on  $\epsilon$ ,

$$\epsilon_{\text{wall}} = 4\nu k_P / d_P^2 - \epsilon_P$$

This is similar to the deduced expression for  $\epsilon$ <sup>8,9</sup> near the wall, although this expression has never been used as a wall boundary condition on  $\epsilon$  to the author's knowledge. Both the expressions due to Refs. 8 and 9, and Ref. 17 were used in the present study. The latter tends to be well behaved, especially in regions of small kinetic energy. This boundary condition provides a self-correcting mechanism in the  $k$  equation through the dissipation term appearing in the source terms for the  $k$ -equation. However, realistic initial profiles for  $k$  and  $\epsilon$  should be provided, otherwise these boundary conditions destabilize the  $k$ - $\epsilon$  system. It is best to start with a zero gradient wall boundary condition on  $\epsilon$ , and switch to this formulation at a later stage in the computations. It is interesting to note that if the zero gradient condition were true, then the boundary condition due to Ref. 9 will be approximately the same as that due to Ref. 17 with wall gradient approximated by the one-sided first order difference formula.

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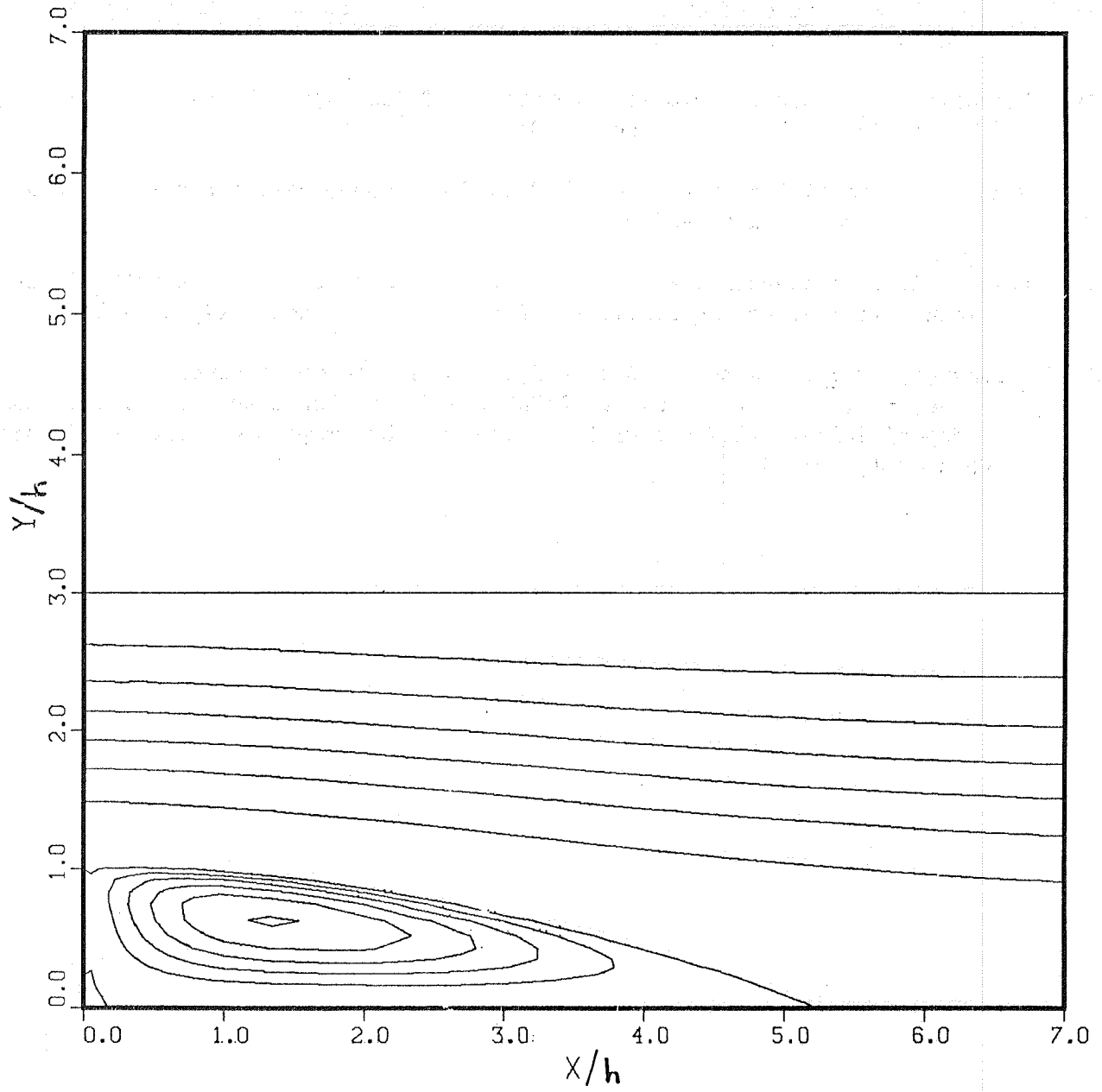


Figure 1.- Stream function contours showing the recirculation zone behind the step.

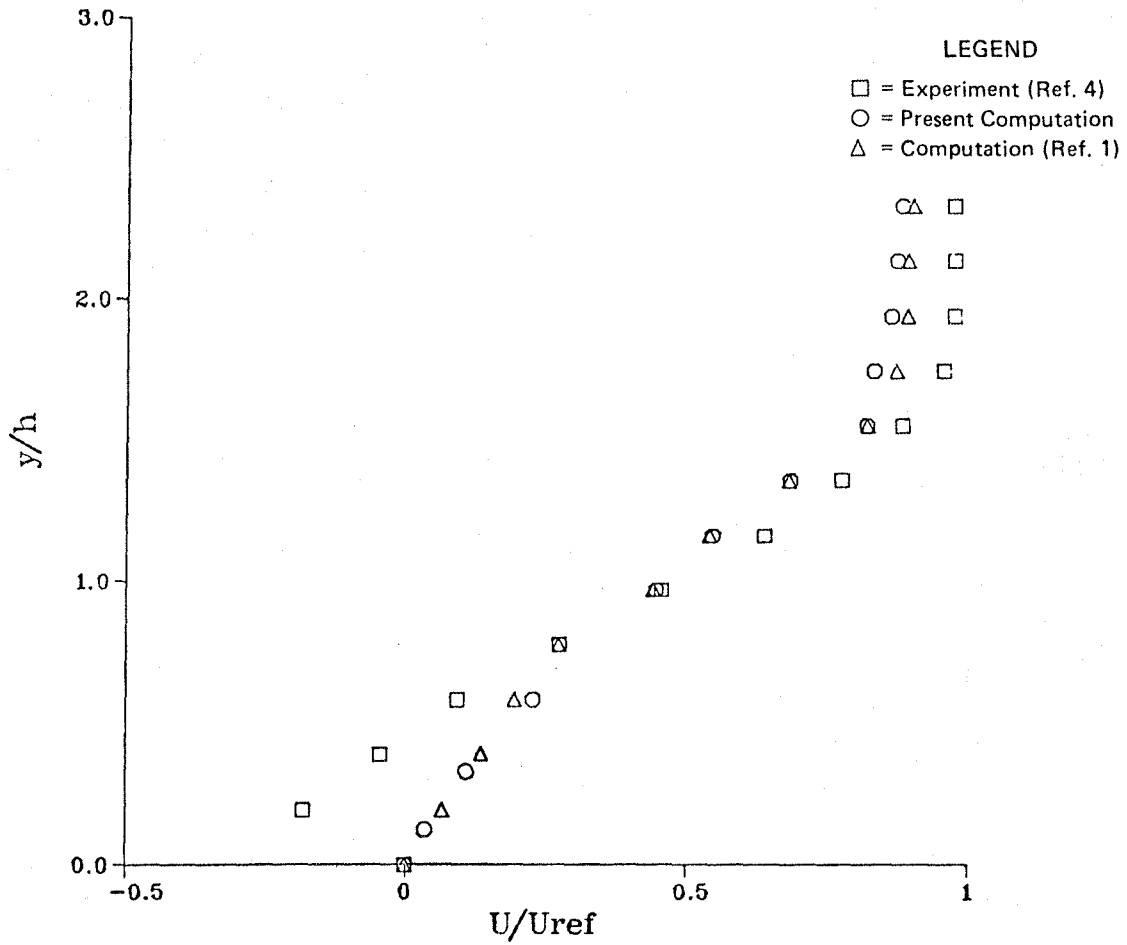


Figure 2.- Mean velocity profile comparison at  $x/h = 5.2$ .

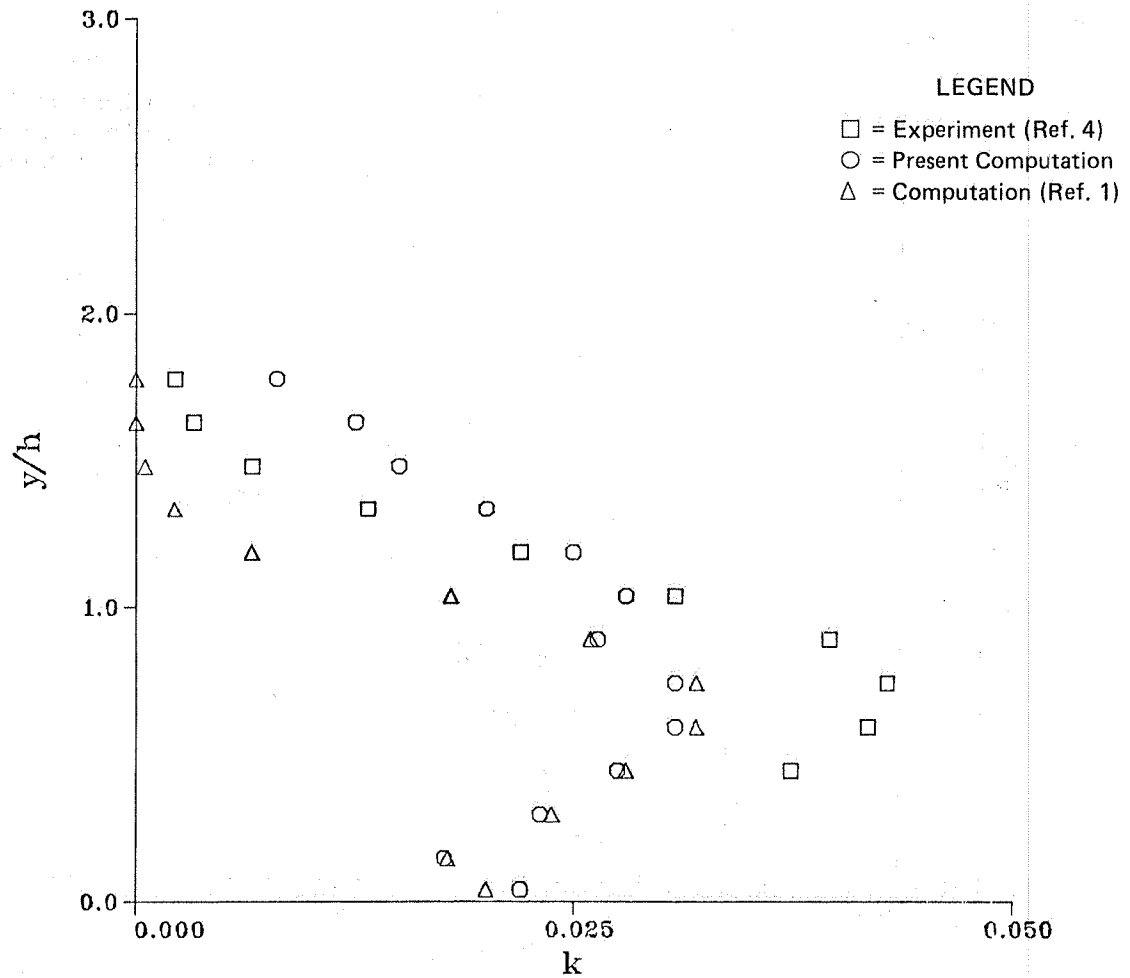


Figure 3.- Comparison of turbulence kinetic energy at  $x/h = 7.7$ .



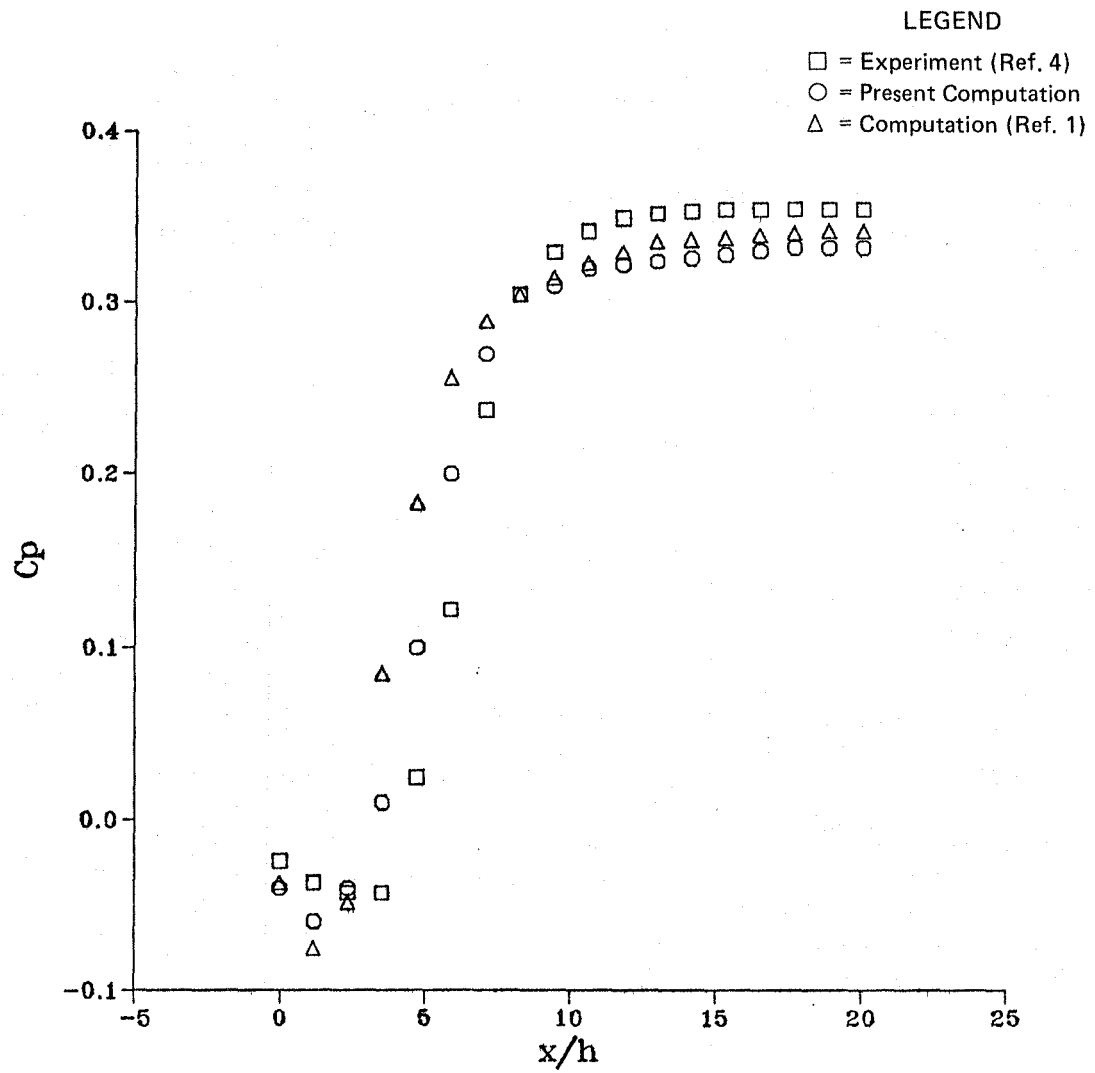


Figure 4.- Comparison of pressure distribution on the step side wall.

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