DEVELOPMENT OF A POSITIVITY–PRESERVING CONVECTION–DIFFUSION–REACTION MODEL FOR TURBULENT QUANTITIES k AND ϵ

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Abstract

In this multi–dimensional flow simulation a composite monotone convection–diffusion–reaction finite element model is developed to discretize constitutive equations for turbulent kinetic energy k and turbulent dissipation rate ϵ. Our goal is to obtain the positive values for k and ϵ solutions based on the M–matrix theory. This paper presents a rigorous validation of the proposed composite model by solving the scalar equations which are amenable to analytic solutions. Then the model is applied to simulate turbulent flows in a lid–driven cavity and in a backward–facing step channel.

Key Words: composite; monotone; convection–diffusion–reaction; turbulent kinetic energy; turbulent dissipation rate; M–matrix theory

1 INTRODUCTION

With comparatively few exceptions, industrial flows are turbulent and one must, therefore, resort to a computationally more challenging turbulent flow simulation. Given an appropriate turbulent model for some turbulent quantities, there exists a difficulty in obtaining physically correct (positive) sign for them. Within the Reynolds hypothesis, a failure to obtain the positive values for k and ϵ will lead to a negative eddy viscosity and, eventually, the divergent solutions. Development of a positivity–preserving numerical model is, thus, the subject of present research.

Use of conventional upwind schemes can stabilize the discretized Navier-Stokes equations but fails to render the positive–valued solution under all circumstances. This is the motivation for the present positivity–preserving approach, which is developed using the M–matrix theory [1, 2]. Given a positive–valued initial solution, the time evolving solution computed from the M-matrix equations will remain positive. In this study, a two–dimensional monotone convection–diffusion-reaction (CDR) finite element model to solve for k and ϵ is developed.

The reminder of this paper is organized as follows. In Section 2 the Reynolds–averaged Navier–Stokes equations, which are solved together with the transport equations for k and ϵ are presented. Then the finite element model for incompressible Navier–Stokes equations are presented. Section 4 deals with the finite element model for solving the constitutive equations for k and ϵ in the two–dimensional domain. The underlying M–matrix theory, which enables calculation of monotone solutions, is also briefly introduced. Section 5 shows some benchmark tests for the validity of the proposed composite numerical model. Concluding remarks are presented in Section 6.

2 WORKING EQUATIONS

The velocity vector $\underline{u}\ (\underline{x}, t)$ and pressure $p\ (\underline{x}, t)$ for a fluid flow with positive viscosity are sought in $\Omega \subset R^d\ (d = 2)$ from the following equations:

$$\underline{u} \cdot \nabla \underline{u} = -\nabla p + \frac{1}{\rho}\ \nabla \cdot \left[\mu_{\text{eff}}(\nabla \underline{u}^T)\right], \qquad (1)$$

$$\nabla \cdot \underline{u} = 0\,. \qquad (2)$$

In the above incompressible flow equations, μ_{eff} denotes the effective viscosity. The piecewise smooth boundary of a simply connected domain is decom-

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posed into Γ_g and Γ_h such that $\Gamma = \Gamma_g \bigcup \Gamma_h$ and $\Gamma_g \bigcap \Gamma_h = \{0\}$. The above elliptic differential system is closed by specifying $\underline{u} = \underline{g}$ at Γ_g or $-p\ \underline{n} + \mu_{\text{eff}} \frac{\partial \underline{u}}{\partial \underline{n}} = \underline{f}_{\text{traction}}$ at Γ_h. Here, $\underline{n}$ is the outward–directed unit vector normal to Γ_h. Provided that Γ_h is empty, existence of solutions requires $\int_\Gamma \underline{g} \cdot \underline{n}\ d\Gamma = 0$.

Given a plausible set of boundary conditions, the primitive variables $\underline{u}$ and p can be calculated from the direct Navier–Stokes simulation provided that the mesh sizes can cover the whole spectrum of eddies. This is hardly ever the case in practice. We will, therefore, resort to the eddy viscosity hypothesis in this study.

Denote μ_{eff} as the sum of the laminar viscosity μ and the turbulent viscosity μ_t, i.e., $\mu_{\text{eff}} = \mu + \mu_t$. The turbulent viscosity μ_t can be expressed in terms of k and ϵ as

$$\mu_t = C_\mu\ \rho\ \frac{k^2}{\epsilon}\ . \tag{3}$$

The constant C_μ shown in the above equation is, to a large majority, chosen to be 0.09. We shall, in what follows, solve for the turbulent kinetic energy k from the following convection–diffusion–reaction (CDR) differential equation:

$$\nabla \cdot (\underline{u}\ k) - \frac{1}{\rho}\ \nabla \cdot \left[(\mu + \frac{\mu_t}{\sigma_k})\ \nabla k \right] + \frac{C_\mu}{\mu_t}\ \rho\ k^2 = \frac{\mu_t}{\rho}\ \mathbf{P}, \tag{4}$$

where $\mathbf{P}\left(\equiv \nabla \underline{u} : (\nabla \underline{u} + \nabla \underline{u}^T)\right)$ is the kinetic energy production. The other turbulent field variable, known as the turbulent dissipation rate ϵ, is also modelled by the following convection–diffusion equation with the quadratic production term

$$\nabla \cdot (\underline{u}\ \epsilon) - \frac{1}{\rho}\ \nabla \cdot \left[(\mu + \frac{\mu_t}{\sigma_\epsilon})\ \nabla \epsilon \right] + C_{\epsilon 2}\ \frac{\epsilon^2}{k} = C_{\epsilon 1}\ C_\mu\ k\ \mathbf{P}. \tag{5}$$

Following Launder and Spalding [3], we set $\sigma_k = 1.0$, $\sigma_\epsilon = 1.3$, $C_{\epsilon 1} = 1.44$ and $C_{\epsilon 2} = 1.92$.

It is important to note that the solutions k and ϵ obtained from the above chosen two constitative equations should, in theory, be positive [4]. The purpose of this study is, thus, to develop a positivity–preserving finite element model since the simulated negative k and ϵ can slow down convergence towards the final solution. Moreover, the erroneous negative eddy viscosity may, in turn, lead to breakdown of calculation.

3 FINITE ELEMENT MODEL FOR THE FLOW EQUATIONS

Consider an admissive function $\underline{w} \in H_0^1(\Omega) \times H_0^1(\Omega)$, where the Hilbert space $H_0^1(\Omega)$ $(=\{l \in H^1(\Omega); l = 0$ on $\partial\Omega\})$ has square–integratable first–order derivatives and a pressure mode $q \in L^2(\Omega)/R$ $(\equiv P)$ (where the quotient space consists of its equivalent class of $L_2(\Omega)$–functions). The weak solutions $(\underline{u},\ p) \in V \left(\equiv H_0^1(\Omega) \times H_0^1(\Omega) \times P\right)$ to equations (1–2) are sought from the following weighted residual equations:

$$\int_\Omega (\underline{u} \cdot \nabla)\underline{u} \cdot \underline{w}\ d\underline{x} + \frac{1}{Re} \int_\Omega \nabla \underline{u} : \nabla \underline{w}\ d\underline{x} - \int_\Omega p \nabla \cdot \underline{w}\ d\underline{x} = \int_\Omega \underline{f} \cdot \underline{w}\ d\underline{x}\ , \forall \underline{w} \in H, \tag{6}$$

$$\int_\Omega (\nabla \cdot \underline{u})\ q\ d\underline{x} = 0,\ \forall q \in P. \tag{7}$$

The test function $\underline{w}$ shown in (6) is constructed by adding the following B^i to the basis functions to construct the Petrov–Galerkin model:

$$B^i = \tau N^j \widetilde{V}_k^{\,j} \frac{\partial N^j}{\partial x_k} \tag{8}$$

The resulting upwind model can yield non–oscillating velocities for the cases where convection prevails, but, at the same time, deteriorate the prediction accuracy due to the false diffusion error [5]. The deteriorated accuracy is particularly severe when grid lines and flow directions are not well aligned. For this reason, a streamline operator is designed to reduce the cross–wind diffusion error in a domain covered by bi–quadratic elements. To avoid oscillatory pressures in the present mixed formulation for incompressible fluid flows, the inf–sup stability condition [6] is enforced by using the bi–quadratic and bi–linear polynomials for the shape functions $N(\underline{x})$ (for the velocity vector) and $M(\underline{x})$ (for the pressure).

By substituting the chosen test and basis equations into equations (6–7), we can derive the following matrix equation in an element Ω^h:

$$\left[\int_{\Omega^h} \left\{ \begin{array}{ccc} C^{ij} & 0 & -M^j \frac{\partial N^i}{\partial X_1} + B^i \frac{\partial M^j}{\partial X_1} \\ 0 & C^{ij} & -M^j \frac{\partial N^i}{\partial X_2} + B^i \frac{\partial M^j}{\partial X_2} \\ M^i \frac{\partial N^j}{\partial X_1} & M^i \frac{\partial N^j}{\partial X_2} & 0 \end{array} \right\} \mathrm{d}\Omega^h \right] \times \begin{pmatrix} u_j \\ v_j \\ p_j \end{pmatrix} = \underline{0}\ . \tag{9}$$

In the above, C^{ij} is expressed as

$$C^{ij} = (N^i + B^i) N^j \widetilde{V}^j_k \frac{\partial N^j}{\partial x_k} + \frac{1}{Re} \frac{\partial N^i}{\partial x_k} \frac{\partial N^j}{\partial x_k} - \frac{1}{Re} B^i \frac{\partial^2 N^j}{\partial x_k \partial x_k} . \quad (10)$$

In the current finite element formulation, τ is derived to obtain a nodally exact solution for the convection–diffusion equation $u\ \phi_x - \frac{1}{Re}\ \phi_{xx} = 0$. In each quadratic element, τ can be derived as [7]

$$\tau(\gamma_\xi) = \begin{cases} \alpha(h_{\tau l}, \gamma_l) & \text{at end-nodes,} \\ \beta(\gamma) & \text{at center-nodes,} \end{cases} \quad (11)$$

where $h_{\tau l} = h_\tau / h_{\tau l}, \gamma_l = u_e h_l Re/2, \gamma = u_c h Re/2$ and

$$\begin{aligned} \alpha(h_{\tau l}, \gamma_l) = & \\ \Big[& -(h_{\tau l} + h_{\tau l}\gamma_l) e^{-2\gamma_l} + 4(2h_{\tau l} + h_{\tau l}\gamma_l) e^{-\gamma_l} \\ & - 7(h_{\tau l} + 1) + 4(2 - h_{\tau l}\gamma_l) e^{h_{\tau l}\gamma_l} \\ & - (1 - h_{\tau l}\gamma_l) e^{2h_{\tau l}\gamma_l} \Big] \\ / \Big[& -(6h_{\tau l} - h_{\tau l}\gamma_l) e^{-2\gamma_l} + 4(3h_{\tau l} - 2h_{\tau l}\gamma_l) e^{-\gamma_l} \\ & + 14 h_{\tau l}\gamma_l + 6(-h_{\tau l} + 1) - 4(3 + 2h_{\tau l}\gamma_l) e^{h_{\tau l}\gamma_l} \\ & + (6 + h_{\tau l}\gamma_l) e^{2h_{\tau l}\gamma_l} \Big] , \end{aligned} \quad (12)$$

$$\beta = \frac{1}{2} \coth(\frac{\gamma}{2}) - \frac{1}{\gamma} . \quad (13)$$

4 CONVECTION–DIFFUSION–REACTION FINITE ELEMENT MODEL FOR k AND ϵ

In this section a positivity–preserving convection–diffusion–reaction finite element model for k and ϵ is developed in bi–linear elements is described. To simplify matters, the following steady–state model equation is considered

$$u\ \Phi_x + v\ \Phi_y - \nu\ (\Phi_{xx} + \Phi_{yy}) + c\ \Phi = f. \quad (14)$$

As an illustrative example, we will study the constant coefficient case in which $c \geq 0$.

The Legendre–polynomials $P_0(t)(\equiv 1)$ and $P_1(t)(\equiv t)$ are used to span the bi–linear weighting and basis functions

$$\begin{aligned} W_i(\xi, \eta) = & D_i\ [d_{\xi_0} P_0(\xi) + d_{\xi_1} P_1(\xi)] \\ & [d_{\eta_0} P_0(\eta) + d_{\eta_1} P_1(\eta)], \end{aligned} \quad (15)$$

$$N_i(\xi, \eta) = \frac{1}{4}\ [P_0(\xi) + \xi_i P_1(\xi)]\ [P_0(\eta) + \eta_i P_1(\eta)]. \quad (16)$$

The five coefficients involved in equation (15) are given in [8]. Using the above Legendre polynomials P_0 and P_1, one can save computing time due to the orthogonal property as given below:

$$\int_{-1}^{+1} P_i(t) P_j(t) dt = \frac{2}{2i+1} \delta_{i,j} \quad (17)$$

where i is dummy index.

The upwind Petrov–Galerkin matrix equation for (14) is of an M–matrix type only for the small Peclet number case [9]. Such a conditionally monotonic model is, thus, applicable only to equations that are discretized by very fine grids. Use of this model to obtain the positive ϕ becomes computationally very expensive. Removal of this strict constraint condition motivated us to employ a less accurate but unconditionally monotone finite element model.

Our strategy of developing an accurate monotonic model is to combine the conditionally monotonic finite element model with the characteristic Galerkin model of Rice and Schnipke [10] as

$$A = \alpha\ A|_{\text{characteristic–Galerkin}} + (1 - \alpha)\ A|_{\text{Legendre-polynomial}} . \quad (18)$$

where

$$\begin{aligned} A_{ij}|_{\text{Legendre-polynomial}} & \\ = \int_{\Omega^e} & u\ W_i \frac{\partial N_j}{\partial x} + v\ W_i \frac{\partial N_j}{\partial y} + \nu\ (\frac{\partial W_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial W_i}{\partial y} \frac{\partial N_j}{\partial y}) \\ & + c\ \delta_{ij}\ W_i \sum_{k=1}^{4} N_k \Big]\ d\Omega^e, \end{aligned} \quad (19)$$

$$\begin{aligned} A_{ij}|_{\text{characteristic–Galerkin}} = & C_{ij} \\ + \int_{\Omega^e} & [\nu\ (\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y}) + c\ \delta_{ij}\ N_i \sum_{k=1}^{4} N_k]\ d\Omega^e. \end{aligned} \quad (20)$$

In the above, equation (20) C_{ij} in defined as

$$C_{ij} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -F_p F_n \frac{u_s}{\Delta s} A_f & -(1 - F_n) \frac{u_s}{\Delta s} A_f & \frac{u_s}{\Delta s} A_f & -(1 - F_p) \frac{u_s}{\Delta s} A_f \\ 0 & 0 & 0 & 0 \end{pmatrix} . \quad (21)$$

Referring to Fig. 1, Δs ($\equiv [(x_3 - x')^2 + (y_3 - y')^2]^{1/2}$) represents the length. Other notations shown in matrix C_{ij} are $A_f = \int_{\Omega^e} \sum_{i=1}^{4} N_i d\Omega^e, 0 \square F_p \equiv max\ \{min\ (\frac{F_1}{F_2}, 1), 0\} \square 1, 0 \square F_n \equiv max\ \{min\ (\frac{F_4}{F_3}, 1), 0\} \square 1, F_1 = v(x_3 - x_4) + u(y_4 - y_3), F_2 = v(x_1 - x_4) + u(y_4 - y_1), F_3 = v(x_2 - x_1) + u(y_1 - y_2), F_4 = v(x_2 - x_3) + u(y_3 - y_2)$. The proper use of α has been verified elsewhere [9].

Nodes	L_2-error Norm	Rate of Convergence
5× 5	7.24410698E-04	
11× 11	1.28145027E-04	1.89
21× 21	3.33891575E-05	1.94

Table 1: The computed L_2–error norms for the analytical test problem presented in Section 5.

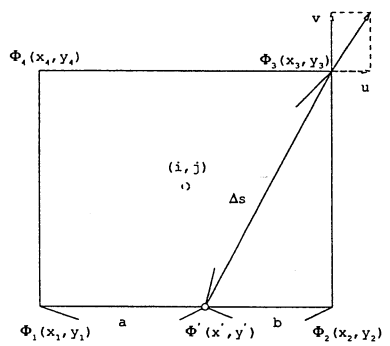


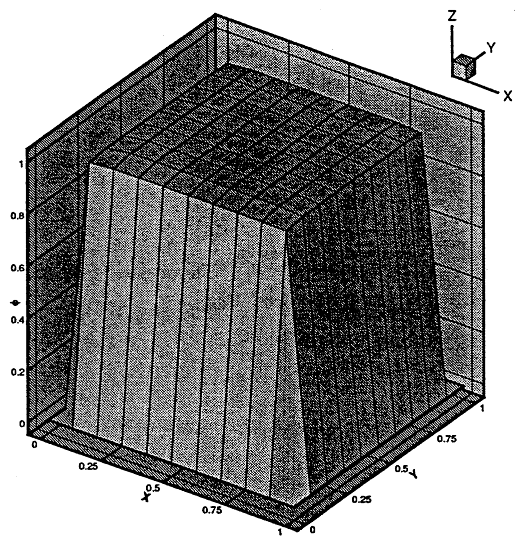
Fig.1: The notations used in the finite element model of Rice and Schnipke.

5 NUMERICAL RESULTS

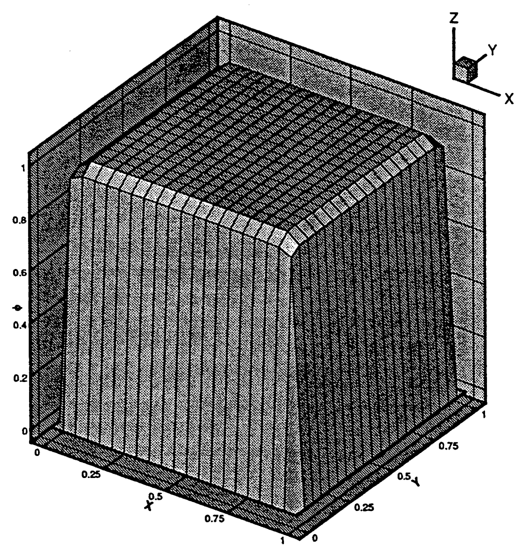
To demonstrate that the proposed finite element model indeed accommodates the positivity–preserving property, the equation (14) in a square $0 \square x \square 1, 0 \square y \square 1$ is considered. For a problem with $u = 1$, $v = 1$, $\nu = 2$, $c = 2$ and $f = 0$, the analytic solution is given by $\Phi = e^{x+y}$. Subject to the analytic boundary condition, finite element solutions are obtained at several continuously refined grid sizes. In Table 1, the simulated L_2–norm errors at 5×5, 11×11 and 21×21 meshes demonstrate the proposed convection-diffusion-reaction finite element model.

A more stringent test case [11] with $f = 1$, $c = 1$, $\nu = 10^{-4}$ and $(u, v) = 10^{-4}(\cos(\pi/3), \sin(\pi/3))$ is considered. Subject to the homogeneous Dirichlet–type boundary condition for Φ, solutions are sought at $\Delta x = \Delta y = 1/10$ and $1/20$. The simulated solutions in Fig. 2 reveal sharp profiles of Φ without any observed oscillations.

Then the lid–driven flow in a square cavity is considered. Based on the lid speed, the length of the cavity, and the kinematic viscosity of the fluid, the Reynolds number for the current study is chosen to be 10000. In this study calculations are performed at $\Delta x = \Delta y = \frac{1}{80}, \frac{1}{120}, \frac{1}{160}$ and 1/256 to obtain grid–independent solutions. It is found from Fig. 3 that the simulated velocity profiles along the centerlines slightly differ from those of Ghia et al. [12]. For the purpose of completeness, the finite element solution at $Re = 4000$ and $\Delta x = \Delta y = \frac{1}{40}$ is plotted. The simu-



(a) $\Delta x = \Delta y = \frac{1}{10}$



(b) $\Delta x = \Delta y = \frac{1}{20}$

Fig.2: The simulated Φ for the investigated Codina problem

lated results in Fig. 4 demonstrate our finite element model, which can render positive values of k, ϵ, and, thus, ν_t even in the vicinity of no–slip wall.

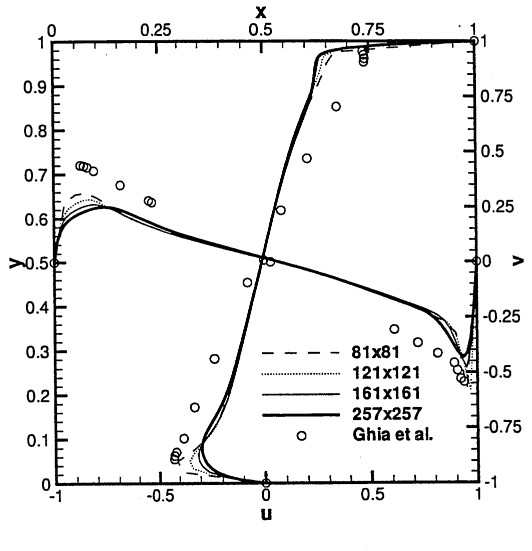


Fig.3: The simulated velocity profiles at Re = 10000 and $\Delta x = \Delta y = \frac{1}{80}, \frac{1}{120}, \frac{1}{160}$ and $\frac{1}{256}$.

Owing to the geometrical simplicity and the availability of experimental data, there was a considerable incentive to study the suddenly expanded channel flow problem. The channel under investigation has a backward–facing step, across which the flow expands into the channel having an expansion ratio of 2. We choose the same flow condition as that of Denham et al. [13] to conduct a direct comparison with the results of physical experiments. For the case with $Re(\equiv u_{\text{mean}} h/\nu) = 3025$, the velocity profiles and $\overline{u'u'}^{1/2}$ are plotted in Figs. 5–6, which exhibit good agreement between the solutions. For completeness, the simulated positive turbulent viscosity μ_t are plotted in Fig. 7.

6 CONCLUDING REMARKS

In this paper a composite finite element model is presented to solve the k and ϵ from the convection–diffusion equation with a quadratic production term. Two upwinding models are used in combination to construct a monotone model at higher Peclet numbers. One finite element model is monotonic when the Peclet number is small. The other finite element model, while is capable of yielding an M–matrix equation for all Peclet numbers, can deteriorate the prediction accuracy in the lower Peclet number case. Therefore, the two models are linearly combined and rigorously de-

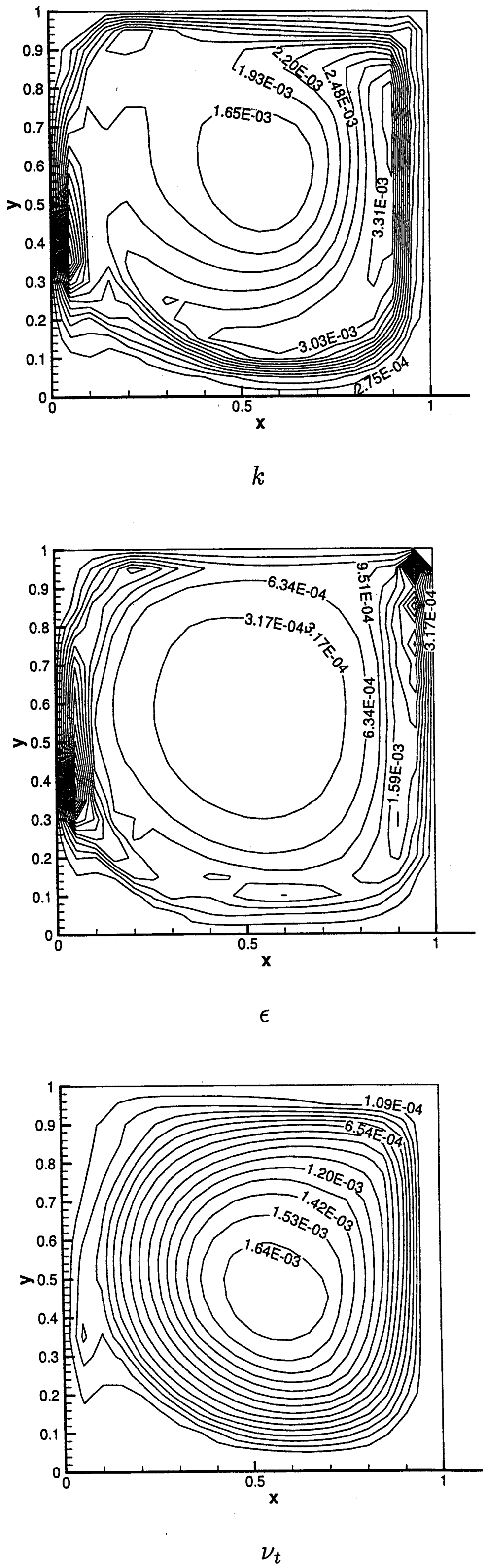


Fig.4: The simulated contours for k, ϵ and ν_t at Re = 4000.

termined the weighting coefficient using the discrete maximum principle. Our aim is to retain high solution accuracy without the loss of stability. Tests using scalar as well as Navier–Stokes equations have been conducted to demonstrate the usefulness of the proposed positivity–preserving composite finite element model.

Acknowledgments

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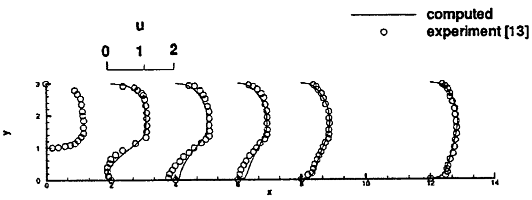

Fig.5: The simulated turbulence intensity profiles at several sections of the channel with a backward facing step.

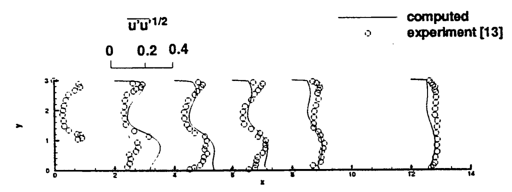

Fig.6: The profiles of the velocity component u at several sections for the backward facing step problem.

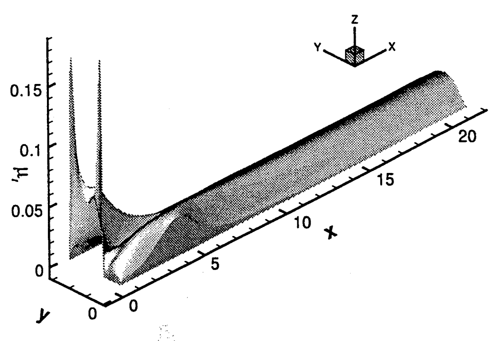

Fig.7: The simulated turbulent viscosity μ_t for the backward facing step problem.

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