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POTENTIAL CAPABILITIES OF REYNOLDS STRESS TURBULENCE MODEL IN THE COMMIX-RSM CODE

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ABSTRACT

A Reynolds stress turbulence model has been implemented in the COMMIX code, together with transport equations describing turbulent heat fluxes, variance of temperature fluctuations, and dissipation of turbulence kinetic energy. The model has been verified partially by simulating homogeneous turbulent shear flow, and stable and unstable stratified shear flows with strong buoyancy-suppressing or enhancing turbulence. This article outlines the model, explains the verifications performed thus far, and discusses potential applications of the COMMIX-RSM code in several domains, including, but not limited to, analysis of thermal striping in engineering systems, simulation of turbulence in combustors, and predictions of bubbly and particulate flows.

INTRODUCTION

The computer code COMMIX-1C [1] describes single-phase, three-dimensional transient thermo-fluid dynamic problems in engineering systems. This code has provided the framework for the extension of the standard k - ϵ turbulence model to a more sophisticated model based on 11 transport equations for the dependent variables describing turbulence: six transport equations for the components of the Reynolds stress tensor, three equations for scalar turbulent heat fluxes, one equation for variance of temperature fluctuations, and one equation for dissipation of turbulence kinetic energy. In isothermal calculations, the system reduces to seven transport equations. The complete Reynolds stress model (RSM) is presented in detail in the next section. A numerical verification of the reduced isothermal system has been made for homogeneous turbulence sustained by a uniform shear in the mean flow. In that case, the governing equations reduce to a system of ordinary differential equations that can be integrated directly, thus providing numerical verification of the code. Moreover, experimental data are available for comparison. The subsequent sections explain ongoing applications of the RSM to stratified flows, which also provide further code verification, and potential applications to several domains of interest for industrial applications where turbulence is highly anisotropic and the standard k - ϵ model therefore performs poorly. The envisaged domains of application include analysis of thermal striping, simulation of turbulence in combustors, and in multicomponent flows.

GOVERNING EQUATIONS FOR REYNOLDS STRESS MODEL

The transport equations for scalar heat fluxes are

$$\frac{\partial}{\partial t}(\overline{u_i \phi}) + U_j \frac{\partial}{\partial x_j}(\overline{u_i \phi}) = \frac{\partial}{\partial x_j} \left[\left(\nu_t + c_{s\phi} \frac{k^2}{\epsilon} \right) \frac{\partial(\overline{u_i \phi})}{\partial x_j} \right] + P_{i\phi} + G_{i\phi} + \pi_{i\phi}. \quad (1)$$

with

$$P_{i\phi} = - \left(\overline{u_i u_j} \frac{\partial T}{\partial x_j} + \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} \right), \quad (2)$$

$$G_{i\phi} = - \beta g_i \overline{\phi^2}, \quad (3)$$

$$\pi_{i\phi} = - c_{1\phi} \frac{\epsilon}{k} \overline{u_i \phi} + c_{2\phi} \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} + c_{3\phi} \beta g_i \overline{\phi^2} - c_{1\phi} \frac{\epsilon}{k} \overline{u_n \phi} \delta_{in} f \left(\frac{L}{x_n} \right). \quad (4)$$

The transport equation for variance of temperature fluctuations is

$$\frac{\partial g}{\partial t} + \frac{\partial (U_j g)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\left(c_\phi \frac{k^2}{\epsilon} + \frac{\lambda}{\rho c_p} \right) \frac{\partial g}{\partial x_j} \right] - \overline{u_j \phi} \frac{\partial T}{\partial x_j} - \frac{\epsilon}{k} \frac{g}{R}. \quad (5)$$

The transport equations for Reynolds stresses are

$$\begin{aligned} \frac{\partial (\overline{u_i u_j})}{\partial t} + U_\ell \frac{\partial (\overline{u_i u_j})}{\partial x_\ell} &= \frac{\partial}{\partial x_\ell} \left[c_k \frac{k^2}{\epsilon} \frac{\partial (\overline{u_i u_j})}{\partial x_\ell} + v_\ell \frac{\partial (\overline{u_i u_j})}{\partial x_\ell} \right] \\ &- (1 - c_2) \left(\overline{u_i u_\ell} \frac{\partial U_j}{\partial x_\ell} + \overline{u_j u_\ell} \frac{\partial U_i}{\partial x_\ell} \right) - \left[\frac{2}{3} \epsilon \delta_{ij} + c_1 \frac{\epsilon}{k} \left(\overline{u_i u_j} - \frac{2k}{3} \delta_{ij} \right) \right] \\ &- \frac{2}{3} c_2 \overline{u_n u_m} \frac{\partial U_n}{\partial x_m} \delta_{ij} - (1 - c_3) \beta (g_i \overline{u_j \phi} + g_j \overline{u_i \phi}) - \frac{2}{3} c_3 \beta g_\ell \overline{u_\ell \phi} \delta_{ij}. \end{aligned} \quad (6)$$

The turbulence kinetic energy is $k = \overline{u_i u_i} / 2$. The transport equation for the dissipation of turbulence kinetic energy ϵ is

$$\begin{aligned} \rho \frac{\partial \epsilon}{\partial t} + \rho U_j \frac{\partial \epsilon}{\partial x_j} &= c_{1\epsilon} \frac{\epsilon}{k} (P_k + G_k) (1 + c_{3\epsilon} R_f) \\ &- c_{2\epsilon} \frac{\rho \epsilon^2}{k} + \frac{\partial}{\partial x_j} \left(\mu_\ell \frac{\partial \epsilon}{\partial x_j} + c_\epsilon \frac{\rho k}{\epsilon} \overline{u_j u_k} \frac{\partial \epsilon}{\partial x_k} \right), \end{aligned} \quad (7)$$

with

APPLICATIONS OF REYNOLDS STRESS MODEL

In this section, we summarize ongoing and potential applications of the RSM in the COMMIX code. The applications involve, but are not limited to, the following fields:

- Stable and unstable stratifications of fluids in engineering systems.
- Thermal striping.
- Turbulence in combustors and in chemically reacting flows.
- Bubbly and particulate flows.

Stable and Unstable Stratifications of Fluids in Engineering Systems

In several engineering systems, including advanced nuclear reactors of the pool type, it is important to analyze the effect of fluid stratifications on turbulence and to predict under which operating conditions natural circulation flows can become established. Because turbulence in stratified flows is highly anisotropic, the standard $k-\epsilon$ model (which assumes isotropy) performs poorly and must be replaced by more sophisticated models, such as the RSM. This domain of applications is exemplified by the two following test cases, which provide further verification of the RSM.

Stratified Shear Flow

An experiment designed to study the effect of buoyancy on turbulent mixing is the case of a horizontal shear flow [5] as sketched in Fig. 1. This figure shows qualitatively the spreading of the region where two fluid streams mix upon entering the domain with different temperatures and velocities. The influence of buoyancy is measured by the reduced Froude number

$$F_r = \frac{|U_2 - U_1|}{\sqrt{g_z \beta h |T_2 - T_1|}}, \quad (10)$$

where the subscript z refers to the vertical component of the gravity acceleration. In stable stratification, when the hot fluid enters at the top, gravity forces oppose the diffusive character of turbulence, which tends to mix the fluids despite their density differences. The smaller the Froude number, the more stable the

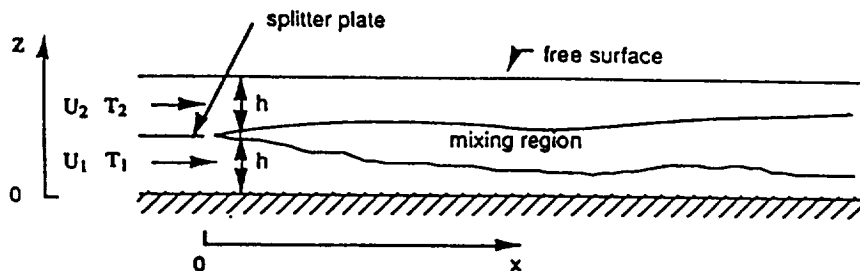


Fig. 1. Sketch of stratified shear flow

$$P_k = \mu_t \left[\frac{\partial U_1}{\partial x_j} \left(\frac{\partial U_1}{\partial x_j} + \frac{\partial U_j}{\partial x_1} \right) \right] \quad (8)$$

$$G_k = -\rho \beta g_i \overline{u_i \phi} \quad (9)$$

The numerical values of the coefficients used in the above equations are as follows: $c_{s\phi} = 0.07$, $c_{1\phi} = 3.1$, $c_{2\phi} = 0.4$, $c_{3\phi} = 0.5$, $c_{1\dot{\phi}} = 0.5$, $c_{\dot{\phi}} = 0.13$, $R = 0.5$, $c_k = 0.09$, $c_1 = 2.8$, $c_2 = 0.47$, $c_3 = 0.4$, $c_{1\epsilon} = 1.44$, $c_{2\epsilon} = 1.92$, $c_{3\epsilon} = 0.8$, $c_\epsilon = 0.15$. Further details about the turbulence model and the boundary conditions used for all transport equations are given in Refs. [2] and [3].

VERIFICATION OF REYNOLDS STRESS MODEL

The RSM has been verified for isothermal homogeneous turbulence maintained by a uniform shear in the mean flow. Homogeneity requires an infinite spatial field that can be simulated numerically by a finite domain with slip-free boundary conditions. Experiments on nearly homogeneous turbulent shear flow have been made in a wind tunnel of height $h = 30.48$ cm and length $L = 10.5 h$ [4]. Turbulence generated by grids at the tunnel entrance becomes almost homogeneous in the center of the tunnel at some distance from the inlet. Measurements were taken in the region defined by $8.5 h \leq x_1 \leq 10.5 h$, x_1 being a coordinate along the horizontal wind tunnel axis. Let x_2 and x_3 be coordinates along a vertical and transverse axis of the tunnel, respectively. In homogeneous turbulence, the mean velocity components of the flow satisfy the conditions $U_1 = U_1(x_2)$; $U_2 = U_3 = 0$; $\partial U_1 / \partial x_2 = \text{constant}$ ($= 13$ in the test case we refer to); $U_2(h/2) = U_c = 12.4$ m/s (center velocity). Under these assumptions, the seven transport equations describing the isothermal flow (Eqs. 6 and 7), reduce to a system of ordinary differential equations that can be integrated directly with the Runge-Kutta algorithm. We made numerical calculations of homogeneous turbulence with the RSM in the COMMIX code and with the Runge-Kutta method in an independent program; we then compared the results with experimental values at $x_1/h = 10$ reported in Ref. [4]. A comparison of computed and experimental results is given in Table I. Under the assumptions made, $\overline{u_1 u_3}$ and $\overline{u_2 u_3}$ are negligibly small. The computed results are much closer to each other than to the experimental values, due to the difficulty of realizing in practice the theoretical conditions of homogeneous turbulence. Theoretically, it must be $\overline{u_2 u_2} = \overline{u_3 u_3}$, a condition satisfied by the results of the calculations but not strictly verified in the experiment. This comparison provides satisfactory verification of the RSM under the given conditions.

Table I. Comparison of experimental and computed turbulence values in homogeneous shear flow

| Turbulence Value | Ref [4] | Runge-Kutta | COMMIX-RSM |
|---|---------|-------------|------------|
| \sqrt{k}/U_c | 0.0185 | 0.0139 | 0.0147 |
| $\sqrt{u_1 u_1}/U_c$ | 0.0178 | 0.0140 | 0.0161 |
| $\sqrt{u_2 u_2}/U_c$ | 0.0132 | 0.0097 | 0.0093 |
| $\sqrt{u_3 u_3}/U_c$ | 0.0141 | 0.0097 | 0.0093 |
| $\sqrt{ u_1 u_2 }/U_c$ | 0.0104 | 0.0101 | 0.0100 |
| $P_k = -\overline{u_1 u_2} \frac{\partial U_1}{\partial x_2}$ | 0.218 | 0.202 | 0.201 |

stratification. Below some threshold of the Froude number, turbulence is completely inhibited by the density gradients. In unstable stratification, when the hot fluid enters at the bottom, the effects of gravity and turbulence combine, forcing a region of highly effective mixing between the hot and cold fluids.

In this study, we used 100 meshes ($\Delta x = 0.03$ m) in the axial direction along the channel length and 30 meshes ($\Delta z = 0.006667$ m) in the transverse direction. The maximum length (x_{\max}) in the x direction is 3 m and the distance ($2h$) between the two plates is 0.2 m. Therefore, the length-to-height ratio (x_{\max}/h) is 30. We present results of a test case with unstable stratification and Froude number 0.9, in which hot water is injected at the lower half of the test section, with $U_1 = U_2/2 = 0.223$ m/s, $T_1 = 128.7^\circ\text{C}$, $T_2 = 20^\circ\text{C}$.

Figure 2 shows the temperature distributions at location $x/h = 20$. With strong mixing, the temperature distributions in hot and cold fluids reach almost the same values. Compared with the $k-\epsilon$ turbulence model, the RSM can produce results closer to the experimental results by accounting for anisotropy of natural circulation and turbulence transport.

Thermal Stratification in a Rectangular Cavity

Thermal stratification experiments have been made in a rectangular cavity filled with liquid sodium and simulating the hot plenum of a liquid-metal fast breeder reactor under steady-state and transient conditions [6]. The cavity communicates at the bottom with a rectangular channel (Fig. 3). A forced flow through the channel induces recirculation in the cavity. In steady-state experiments, temperature differences were induced by heating one wall of the cavity; in transient tests, by decreasing the temperature of the inlet flow.

We simulated one steady-state experiment (referred to as P1 in Ref. [6]). In this test, the inlet flow temperature was 300°C , while the right-hand wall of the cavity was kept at 316°C . Measured and computed vertical normalized temperature profiles in the cavity 200 mm from the left wall are given in Fig. 4. As in the previous test cases, the $k-\epsilon$ model performs poorly, while the RSM results agree fairly well with the experimental ones.

Thermal Striping

Thermal striping is characterized by random temperature fluctuations in regions where flows with different temperatures mix. The temperature fluctuations, with frequency components of 2 to 20 Hz, induce cycle fatigue in structural materials. The problem of analyzing thermal striping and minimizing its impact upon structures is of concern in both nuclear and conventional industries.

Combined buoyancy and striping phenomena have been investigated at ANL in piping, plena, heat exchangers, and steam generators. The distribution of temperature and velocity fields at the point where a horizontal pipe conveying water enters a plenum has been investigated as a function of the temperature difference between pipe inlet and bulk plenum temperature. In particular, the experimental program aimed at investigating (a) the length and height of the stratified recirculating flow carrying fluid from the plenum

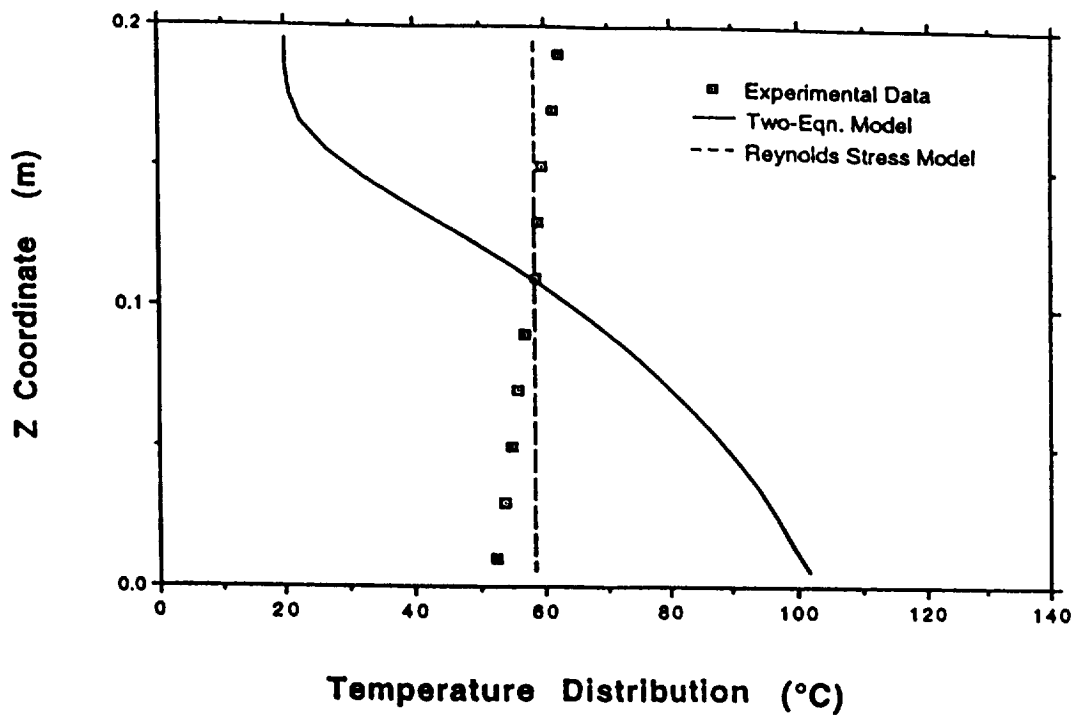


Fig. 2. Temperature distributions for unstable stratified shear flow at $x/h = 20$

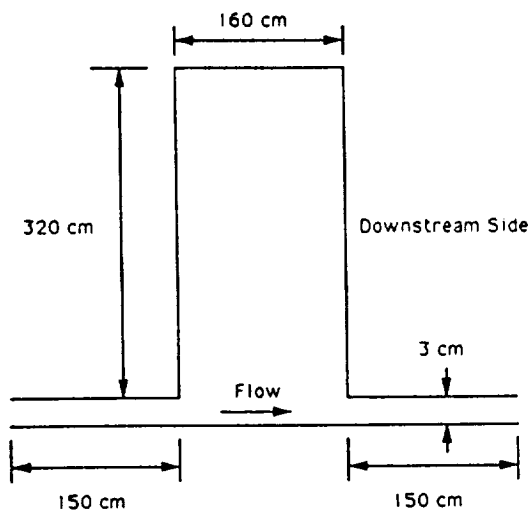


Fig. 3. Sketch of thermal cavity

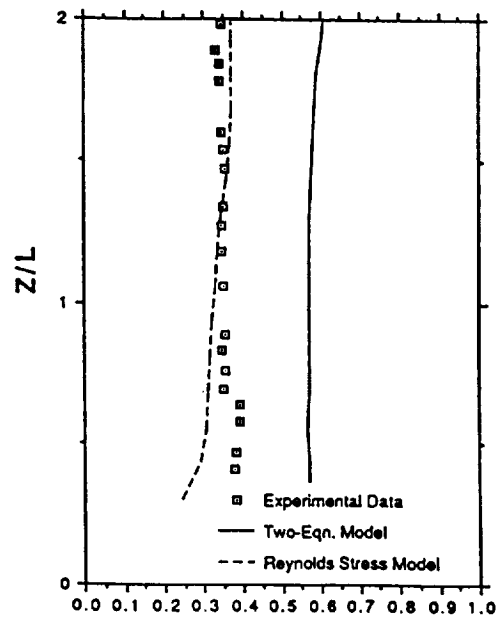


Fig. 4. Measured and computed normalized temperature distributions in the cavity, 200 mm from the left wall

into the pipe; (b) the temperature fluctuations at the pipe walls, hence the potential damage due to thermal striping; and (c) the interaction between the thermal plume and the fluid plenum, hence the buoyancy-generated large-scale eddies in the plenum and the time evolution of plenum temperatures.

Numerical simulations of the flow and temperature fields at the junction between a horizontal pipe conveying hot fluid and a plenum initially filled with cold fluid have been made with the $k-\epsilon$ turbulence model [7]. These computations failed to reproduce correctly the dynamics of the thermal plume in the plenum and the length of cold fluid penetration into the pipe. The latter was underestimated by a factor of 3. Thus, thermal striping analysis in the pipe could only be inferred. These discrepancies are due to the approximate representation of buoyancy forces and to the assumption of isotropy of turbulence inherent in the $k-\epsilon$ model. Both of these limitations are eliminated in the RSM, which is more appropriate for detailed analysis of this and related problems. Numerical simulation of this test case with the RSM is underway at ANL.

Turbulence in Combustors and in Chemically Reacting Flows

Advanced combustion technologies are being developed with the goal of achieving higher overall system efficiencies and reduced environmental loading of air and water with solid pollutants. Further developments tend toward systems combining a pressurized, high-intensity combustor (which produces higher entrainment of the ambient fluid and fast mixing) with gas or steam turbines to optimize cycle efficiency and minimize pollutant formation.

Computation of swirling turbulent flows in which turbulence is nonhomogeneous and anisotropic is a problem of major concern. It has been suggested that the assumptions leading to the formulation of the $k-\epsilon$ model are inadequate for the simulation of turbulence in highly swirling flows [8]. Traditionally, designers have relied on experiments to derive empirical correlations describing heat and mass transfer. The validity of these correlations is generally limited to the experimental conditions for which they have been obtained. This traditional approach can now be supplemented with computational turbulence modeling (e.g., COMMIX-RSM), which gives the designer the predictive capability to change parameters and choose the conditions that lead to improved combustors with higher efficiency and less pollution.

From the standpoint of numerical simulation of combustion involving several chemical components, the state-of-the-art code is KIVA-II [9]; this is the last of a series of programs developed for, but not limited to, applications to internal combustion engines. This code is applicable to a variety of multi-dimensional fluid-dynamic problems with or without chemical reactions. Turbulent flows are computed with either a standard version of the $k-\epsilon$ model or a subgrid scale (SGS) turbulence model in which large-scale eddies are resolved while small scale turbulence is modeled. These models, however, do not account for the presence of particles (e.g., coal particles in coal-fired diesel engines) in the carrying fluid and for the damping of the turbulence kinetic energy due to the presence of particles. Reynolds stress models can be applied to multifield turbulent transport by extending the procedure used for one-fluid turbulence to the several fields and taking into account their interactions [10]. The potential improvement of multiphase turbulence modeling provided by multifield RSM is worthy of consideration, at high computational costs, however.

Bubbly and Particulate Flows

Numerical simulations of bubbly and particulate flows in pipes are of interest for a variety of applications ranging from analysis of blood vessels to material transport by slurry flows. Numerical analysis aims at predicting pressure drops, relative velocity between continuous and particulate phases, and particle concentrations across flow stream lines. Turbulence predictions in the continuous phase have been

made [11] with a standard k - ϵ turbulence model and additional terms that account for the interfacial turbulent momentum transfer. Numerical analysis of turbulent bubbly flow and particulate flow is being carried out at ANL with the same approach as in Ref. [11]. Preliminary results for bubbly flows have been documented in Ref. [3]. The assumption of isotropic turbulence inherent in the k - ϵ turbulence model is however not satisfied in these cases. An extension of the RSM to two phases has been proposed in Ref. [12] and is being planned at ANL, in a way suitable for the numerical simulation of multicomponent flows.

CONCLUSIONS

In all cases where turbulence is anisotropic, and especially when enhancement or suppression of turbulence intensity due to buoyancy forces plays a dominant role, the RSM allows more realistic numerical predictions than the standard k - ϵ model, which is based on the inherent assumption of isotropic turbulence. The RSM can be applied to a variety of domains of interest for technological applications. Its extension to multicomponent flows is possible, at the expense, however, of high computational costs. To cope with these, more advanced solution algorithms for the transport equations and code parallelization are envisaged.

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NOMENCLATURE

| | |
|-------------|---|
| c_p | Specific heat (J/kg-K) |
| F_r | Froude number |
| G_k | Production or suppression of turbulence kinetic energy due to buoyancy (J/s-m ³) |
| $G_{i\phi}$ | Buoyancy production in scalar flux equations (m-K/s ²) |
| g | $\left(= \frac{1}{2} \overline{\phi^2} \right)$, one-half of variance of temperature fluctuations (K ²) |
| \vec{g} | Gravity acceleration (m/s ²) |
| k | Turbulence kinetic energy (m ² /s ²) |
| L | Length scale (m) |
| P_k | Mean shear production in k and ϵ equations (J/s-m ³) |
| $P_{i\phi}$ | Mean field production in scalar flux equations (m-K/s ²) |
| R_f | (= - G_k/P_k), Richardson number |
| T | Temperature (K) |
| t | Time (s) |

- U Mean flow velocity (m/s)
u Fluctuation of velocity (m/s)
 $\overline{u_i \phi}$ Scalar heat flux (m-K/s)
 $\overline{u_i u_j}$ Reynolds stress (m²/s²)
x_i Coordinate direction (m)

Greek

- β $\left[-\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p \right]$, volume expansion coefficient at constant pressure (K⁻¹)
 δ_{ij} Kronecker delta
 ϵ Dissipation of turbulence kinetic energy (W/kg)
 λ Thermal conductivity (W/m-K)
 μ Dynamic viscosity (kg/m-s)
 ν Kinematic viscosity (m²/s)
 $\pi_i \phi$ Pressure-scalar gradient correlation in scalar heat flux equations (m-K/s²)
 ρ Density (kg/m³)
 ϕ Temperature fluctuation (K)
 $\overline{\phi^2}$ Variance of temperature fluctuations (K²)

Indices

- l Laminar
n Normal to wall
t Turbulent

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