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**IMPLEMENTATION AND VALIDATION OF A REYNOLDS STRESS
MODEL IN THE COMMIX-1C/RSM
AND CAPS-3D/RSM CODES**

by

F. C. Chang and M. Bottoni

Energy Technology Division

August 1995

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U.S. DEPARTMENT OF ENERGY
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Nomenclature

A^+	Constant (= 0.025) used in g equation
A_f	Control volume crossflow area (m ²)
a_{ij}	Tensor components defined by Eq. 4.1.1.11
a_{β}^g	Coefficients of g Eq. 3.2.18 ($\beta = 0, 1, 2, \dots, 6$) (kg/s)
a_{β}^h	Coefficient of linearized enthalpy equation, defined by Eq. 4.4.2.8 ($\beta = 0, 1, 2, \dots, 6$) (kg/s)
$a_{\beta}^{\overline{u_i\phi}}$	Coefficients of scalar flux Eq. 3.1.38 ($i = 1, 2, \text{ and } 3$) ($\beta = 0, 1, 2, \dots, 6$) (kg/s)
a_{β}^{ε}	Coefficients of linearized ε equation, defined by Eq. 4.2.2.8 ($\beta = 0, 1, 2, \dots, 6$) (kg/s)
$a_{\beta}^{\Phi_{ij}}$	Coefficients of linearized Reynolds stress equations, defined by Eq. 4.1.2.9 ($\beta = 0, 1, 2, \dots, 6$) (kg/s)
b_0^g	Right-hand side of g Eq. 3.2.18 (kg-K ² /s)
b_0^h	Right-hand side of linearized enthalpy equation, defined by Eq. 4.4.2.8h (W)
$b_0^{\overline{u_i\phi}}$	Right-hand side of scalar flux Eq. 3.1.38 ($i = 1, 2, \text{ and } 3$) (kg-m ^{-°K} /s ²)
b_0^{ε}	Right-hand side of linearized ε equation, defined by Eq. 4.2.2.8h (kg-m ² /s ⁴)
$b_0^{\Phi_{ij}}$	Right-hand side of linearized Reynolds stress equation, defined by Eq. 4.1.2.9h (kgm ² /s ³)
c_g	Constant (= 1.0) used in g equation
c_p	Specific heat (J/kg-K)
c_s	Constant (= 0.09) used in Reynolds stress equations
c_1	Constant (= 2.8), used in Reynolds stress equations
c_2	Constant (= 0.47), used in Reynolds stress equations
c_3	Constant (= 0.47), used in Reynolds stress equations
c_{ε}	Constant (= 0.15), used in ε equation
$c_{1\varepsilon}$	Constant (= 1.44), used in ε equation
$c_{2\varepsilon}$	Constant (= 1.92), used in ε equation
$c_{3\varepsilon}$	Constant (= 0.8), used in ε equation
c_{μ}	Constant (= 0.09), used in scalar flux equations

c'_{ϕ}	Constant (= 0.13), used in g equation
$c_{1\phi}$	Constant (= 3.1), used in scalar flux equations
$c'_{1\phi}$	Constant (= 0.5), used in scalar flux equations
$c_{2\phi}$	Constant (= 0.4), used in scalar flux equations
$c_{3\phi}$	Constant (= 0.5), used in scalar flux equations
$c_{s\phi}$	Constant (= 0.07), used in scalar flux equations
D	Diffusion coefficients, first defined by Eq. 3.1.36 (kg/s)
D_h	Hydraulic diameter (m)
d	Coefficient that multiplies pressure increments in discretized momentum equation. Defined by Eq. 4.3.2.6 (m^2).
E	Constant (= 9.0), used for boundary conditions of Reynolds stress equations
F	Convection coefficients, defined by Eq. 3.1.34 (kg/s)
F_r	Froude number
G_k	Production or suppression of turbulence kinetic energy due to buoyancy (m^2/s^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 the variance of temperature fluctuations (K^2)
g_i	Components of gravitational acceleration ($i = 1, 2, \text{ and } 3$) (m/s^2)
g_w	One-half of the variance of temperature fluctuations at wall (K^2)
H	Height between two horizontal plates (m)
J_g	$\left(= J_g^c + J_g^d\right)$ Total (convective plus diffusive) flux in g equation ($m-K^2/s$)
J_g^c	Convective flux in g equation ($m-K^2/s$)
J_g^d	Diffusive flux in g equation ($m-K^2/s$)
$\tilde{J}_{\phi}$	$\left(= J_{\phi}^c + J_{\phi}^d\right)$ Total (convective plus diffusive) flux in scalar flux equation (m^2-K/s^2)
J_{ϕ}	$\left(= \rho \tilde{J}_{\phi}\right)$ Total flux times density in scalar flux equation ($K\text{-kg}/m\text{-s}^2$)
J_{ϕ}^c	Convective flux in scalar flux equations (m^2-K/s^2)
J_{ϕ}^d	Diffusive flux in scalar flux equations (m^2-K/s^2)
J_{hj}	$\left(= J_{hj}^c + J_{hj}^{d\ell} + J_{hj}^{dt}\right)$ Total (convective plus diffusive) flux in enthalpy equation, defined by Eq. 4.4.1.6 (W/m^2)

- J_{hj}^c ($= \rho u_j h$) Convective flux in enthalpy equation, defined by Eq. 4.4.1.3 (W/m²)
- $J_{hj}^{d\ell}$ $\left(= -\frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} \right)$ Laminar diffusive flux in enthalpy equation, defined by Eq. 4.4.1.4 (W/m²)
- J_{hj}^{dt} ($= \rho c_p \overline{u_j \phi}$) Turbulent diffusive flux in enthalpy equation, defined by Eq. 4.4.1.5 (W/m²)
- $J_{\epsilon j}$ ($= J_{\epsilon j}^c + J_{\epsilon j}^{d\ell} + J_{\epsilon j}^{dt}$) Total (convective plus diffusive) flux in ϵ equation defined by Eq. 4.2.1.9 (kg/s⁴)
- $J_{\epsilon j}^c$ ($= \rho u_j \epsilon$) Convective flux in ϵ equation, defined by Eq. 4.2.1.5 (kg/s⁴)
- $J_{\epsilon j}^{d\ell}$ $\left(= -\mu_\ell \frac{\partial \epsilon}{\partial x_j} \right)$ Laminar diffusive flux in ϵ equation, defined by Eq. 4.2.1.6 (kg/s⁴)
- $J_{\epsilon j}^{dt}$ $\left(= -\Gamma_{\epsilon j} \frac{\partial \epsilon}{\partial x_m} \right)$ Turbulent diffusive flux in ϵ equation, defined by Eq. 4.2.1.7 (kg/s⁴)
- J_{mij} ($= J_{mij}^c + J_{mij}^{d\ell} + J_{mij}^{dt}$) Total (convective plus diffusive) flux in momentum equation, defined by Eq. 4.3.1.5 (kg/m-s²)
- J_{mij}^c ($= \rho U_i U_j$) Convective flux in momentum equation, defined by Eq. 4.3.1.2 (kg/m-s²)
- $J_{mij}^{d\ell}$ $\left(= -\mu_\ell \frac{\partial U_i}{\partial x_j} \right)$ Laminar diffusive flux in momentum equation, defined by Eq. 4.3.1.3 (kg/m-s²)
- J_{mij}^{dt} ($= \rho \overline{u_i u_j}$) Turbulent diffusive flux in momentum equation, defined by Eq. 4.3.1.4 (kg/m-s²)
- K ($= 0.42$), von Karman constant
- k Turbulent kinetic energy (J/kg)
- L Length scale (m)
- P_g $\left(= \frac{1}{2} P_\phi \right)$ Mean field production in g equation (K²/s)
- P_{ij} Stress production due to mean flow (m²/s³)
- P_k Mean shear production in k and ϵ equations (m²/s³)
- $P_{i\phi}$ Mean field production in scalar flux equations ($i = 1, 2$, and 3) (m-K/s²)
- Pr Prandtl number
- p Pressure (N/m²)
- q_w Heat flux from surface [J/(s-m²)]
- R Constant ($= 0.5$) used in g equation

R_f	(= $-G_k/P_k$), Richardson number
R_i	Components of friction forces in momentum equation ($\text{kg/m}^2\text{-s}^2$)
S_g	Source term in g equation (K^2/s)
S_h	Source term in enthalpy equation (W/m^3)
S_{ij}^L	Source term in Reynolds stress equations, defined by Eq. 4.1.2.6 (m^2/s^3)
S_{ij}^R	Source term in Reynolds stress equations, defined by Eq. 4.1.2.5 (m^2/s^3)
S_{mi}	Source term in momentum equations, defined by Eq. 4.3.1.6 ($\text{kg/m}^2\text{-s}^2$)
S_ϵ	Source term in ϵ equation, defined by Eq. 4.2.1.3 (kg/m-s^4)
$S_{\phi i}$	Source term in scalar flux equations ($i = 1, 2, \text{ and } 3$) (m-K/s^2)
T	Temperature (K)
T_w	Wall temperature (K)
U_i	Components of mean velocity ($i = 1, 2, \text{ and } 3$) (m/s)
u_i	Fluctuation of velocity component ($i = 1, 2, \text{ and } 3$) (m/s)
u_n	Fluctuation of velocity component normal to the wall (m/s)
u^*	Friction velocity (m/s)
$\bar{u}$	Mean velocity at inlet (m/s)
$\overline{u_i \phi}$	(= Φ) Scalar flux ($i = 1, 2, \text{ and } 3$) (m-K/s)
$\overline{u_i u_j}$	Reynolds stress (m^2/s^2)
V_f	Fluid volume in a control cell (m^3)
x_i	Coordinate ($i = 1, 2, \text{ and } 3$) (m)
x_n	Distance from the wall (m)
x^*	(= x/D_h) Axial coordinate normalized to the hydraulic diameter
y_ℓ	Thickness of laminar sublayer (m)
y_ℓ^+	Dimensionless thickness of laminar sublayer
y_p	Distance of node P from the wall (m)

Greek

β	$\left[= -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p \right]$ Volume expansion coefficient at constant pressure (K^{-1})
---------	--

γ	Surface permeability
Γ_g	Total (laminar plus turbulent) diffusivity in g equation (m^2/s)
$\Gamma_{g\ell}$	$\left(= \frac{\lambda}{\rho c_p} \right)$ Laminar diffusivity (m^2/s)
Γ_{gt}	$\left(= c_\phi \frac{k^2}{\varepsilon} \right)$ Turbulent diffusivity (m^2/s)
$\Gamma_{\Phi ij}$	$\left(= \nu_\ell + c_s \frac{k^2}{\varepsilon} \right)$ Diffusion coefficient in Reynolds stress equations (m^2/s)
Γ_ϕ	$\left(= \rho \Gamma_\phi^v = \mu_\ell + \rho c_{s\phi} \frac{k^2}{\varepsilon} \right)$ Total (laminar plus turbulent) dynamic diffusivity in scalar flux equations ($\text{kg}/\text{m-s}$)
Γ_ϕ^v	$\left(= \nu_\ell + c_{s\phi} \frac{k^2}{\varepsilon} \right)$ Total (laminar plus turbulent) kinematic diffusivity in scalar flux equations ($\text{kg}/\text{m-s}$)
$\Gamma_{\varepsilon jm}$	$\left(= c_\varepsilon \rho \frac{k}{\varepsilon} \overline{u_j u_m} \right)$ Turbulent diffusion coefficient in ε equation, defined by Eq. 4.2.1.8 ($\text{kg}/\text{m-s}$)
δ	Unity vector
δ_{ij}	Kronecker delta
Δl	Length (m)
ε	Dissipation of turbulent kinetic energy (W/kg)
ε_g	$\left(= \frac{1}{2} \varepsilon_\phi \right)$ Dissipation in g equation (K^2/s)
λ	Thermal conductivity ($\text{W}/\text{m-K}$)
μ_{eff}	Effective dynamic viscosity ($\text{kg}/\text{m-s}$)
μ	Dynamic viscosity ($\text{kg}/\text{m-s}$)
ν	Kinematic viscosity (m^2/s)
π_{ij}	Pressure strain tensor ($\text{m-K}/\text{s}^2$)
$\pi_{i\phi}$	Pressure-scalar gradient correlation in scalar flux equations ($\text{m-K}/\text{s}^2$)
$\pi_{i\phi}^w$	Wall contribution to pressure-scalar gradient correlation in scalar flux equation ($\text{m-K}/\text{s}^2$)
ρ	Density (kg/m^3)

σ_t	(= 0.9) Turbulence Prandtl number for heat transport, used in scalar flux equations
σ_ϕ	Constant (= 1.3) used in scalar flux equations
Φ_{ij}	Components of Reynolds stress tensor (m^2/s^2)
ϕ	Temperature fluctuation (K)
$\overline{\phi^2}$	Variance of temperature fluctuation (K^2)

Indices

c	Convective
d	Diffusive
i,j,k	Free or dummy indices
ℓ, m, n	Free or dummy indices
f	Fluid
ℓ	Laminar
m	Momentum
n	Normal to wall
n	Time discretization level
o	Inlet/central node
p	Node P
t	Turbulent
w	Wall
α, β	Dummy indices

Special Symbols

[a, b]	max (a, b)
∇	Gradient
$\nabla \cdot$	Divergence
$\bullet$	Scalar product
$:$	Double dot product

Implementation and Validation of a Reynolds Stress Model in the COMMIX-1C/RSM and CAPS-3D/RSM Codes

F. C. Chang and M. Bottoni

Abstract

A Reynolds stress model (RSM) of turbulence, based on seven transport equations, has been linked to the COMMIX-1C/RSM and CAPS-3D/RSM computer codes. Six of the equations model the transport of the components of the Reynolds stress tensor and the seventh models the dissipation of turbulent kinetic energy. When a fluid is heated, four additional transport equations are used: three for the turbulent heat fluxes and one for the variance of temperature fluctuations. All of the analytical and numerical details of the implementation of the new turbulence model are documented. The model was verified by simulation of homogeneous turbulence.

Executive Summary

This report first explains the details of the well-known problem of the poor performance of the k - ϵ turbulence model in fluid-dynamic calculations when the flow is thermally stratified and when there are recirculating stream patterns. To cope with this problem, the production or suppression of turbulent kinetic energy due to buoyancy forces, and the components of the Reynolds stress tensor must be computed rigorously.

Because buoyancy forces depend on thermal fluxes, it is necessary to correctly compute these fluxes by numerically solving the respective transport equations in the three coordinate directions. These equations, in turn, depend on the variance of temperature fluctuations that thus requires a fourth transport equation. The intensity of the Reynolds stresses $\overline{u_i u_j}$ is governed by six transport equations. A seventh equation is needed for the dissipation of turbulent kinetic energy ϵ . In the last equation, the turbulence diffusion term must be compatible with the diffusion terms used in the Reynolds stress equations. Thus, the ϵ equation used in combination with the Reynolds stress model (RSM) is different from the equation used in the k - ϵ model.

The full RSM thus consists of 11 transport equations. The report explains modeling of these equations from the most general formulation to the form used for the linearization, which yields a discrete Poisson-like equation for the transported physical quantity.

In addition to explaining the 11 equations of the RSM, the report explains the analytical and numerical treatment of the momentum and enthalpy equations for fluid flow.

These equations are different from those used in the k - ϵ model because turbulent viscosity and conductivity are replaced by Reynolds stresses and turbulent heat fluxes, respectively.

The model is numerically verified by simulating homogeneous turbulence and the results of the verification can be compared with experimental data.

1 Introduction

Complex turbulent flows exist in many engineering applications and industrial environments. For example, turbulent flows occur in the wakes of submarines, in the boundary layers growing on aircraft wings, in combustion processes, and in the flows of natural gas and oil in pipelines. The study of turbulence clearly is an interdisciplinary activity that has a very wide range of applications.

Although the Navier-Stokes equations can properly describe turbulent motion, it is too costly and time consuming for engineers to solve them in complex situations. Instead, ensemble-averaged Navier-Stokes equations are often sufficient to describe turbulent phenomena. However, in taking the average of the Navier-Stokes equations for turbulent flow, which is three-dimensional, unsteady, irregular, and rotational, detailed information on fluid motion is lost. To cope with this disadvantage, a turbulence model must be introduced.

The standard k - ϵ two-equation model has been implemented in the COMMIX-1C code.^{1,2} Subsequent work has introduced a turbulence model that accounts for the anisotropy of turbulence in flow situations characterized by strong buoyancy forces. The first motivation for this development came from safety analyses of nuclear reactors.

Inherent safe operation of the reactor was one of the most important features of the proposed integral fast reactor (IFR). This passive safety feature can be achieved by natural circulation as a result of thermal stratification in the reactor system. Even in the worst case of loss of power to the primary pumps, natural circulation must provide, through intermediate heat exchangers, a heat sink that can prevent coolant temperatures from reaching saturation and triggering local boiling, with subsequent reduction in cooling capabilities and loss of core integrity. Therefore, accurate prediction of temperature distribution in a reactor system that is in a natural-circulation environment was of paramount importance for the IFR.

Because natural-circulation phenomena are not isotropic, there was a need to develop an anisotropic turbulence model (ATM) that could be used to predict more accurately the effects of natural circulation on the reactor system. It was also necessary to model the impact of stratification of coolant temperature on turbulence, an impact that can be enhanced or suppressed according to stable or unstable stratification patterns in a reactor pool.

The ATM became available in the COMMIX-1C/ATM version of the code.³ The ATM is based on three scalar equations for the fluxes, on one equation for the variance of

temperature fluctuations, and on two equations for k and ϵ . Therefore, six scalar turbulence transport equations are involved.

The development of the ATM helped to refine the interaction between turbulence phenomena and buoyancy forces and accounted for the effect of temperature and velocity fluctuations on transport of turbulence. However, in the course of verifying the ATM against experimental data, it became evident that a rigorous computation of Reynolds stresses was necessary. These stresses appear in the equations for the turbulent scalar fluxes and also replace the turbulent viscosity in the momentum equations. Likewise, the turbulent scalar fluxes replace turbulent conductivity in the enthalpy equation of the fluid.

With the computation of the six Reynolds stresses, and dropping the k equation, which becomes superfluous, the full Reynolds stress model (RSM) consists of 11 transport equations.

Section 2 of this report states more clearly the need for an advanced turbulence model for thermo-fluid-dynamic calculations. The analytical and numerical treatments of the equations for turbulent heat fluxes and for the variance of temperature fluctuations is presented in Sec. 3. All of the details of the RSM proper, namely of the transport equations for $u_i u_j$, are given in Sec. 4. A synopsis of the full model is given for ease of reference in Sec. 5. Finally, the verification of the model against experimental data is illustrated in Sec. 6. The 11-equation RSM has been implemented in an updated version of the COMMIX-1C code, referred to as COMMIX-1C/RSM and in the CAPS-3D/RSM code,⁴ which is used for numerical simulation of casting problems.

2 The Need for a Reynolds Stress Model. Statement of the Problem

In the safety analysis of advanced fast breeder reactors, licensing authorities require that inherent safety capabilities be proved by numerical simulation with well-validated computer programs. Even in the worst case of loss of power to the primary pump, natural-convection circulation must provide, through intermediate heat exchangers, a heat sink that can prevent coolant temperatures from reaching saturation and triggering development of a two-phase flow domain with subsequent reduction of coolant capabilities and loss of core integrity.

This approach, based on inherent (or passive) reactor safety, was being followed in the development of the IFR at Argonne National Laboratory. Numerical simulations of reactor coolant behavior require the modeling of turbulent flows in the critical transition phase between forced and natural convection. It is also necessary to model the impact of stratification of coolant temperature on turbulence, an impact that can be enhanced or suppressed according to unstable or stable stratification patterns.

In the critical transition phase between forced and natural convection, however, turbulence models based on two equations, like the k - ϵ model, are inadequate because they assume isotropic behavior of turbulence, an assumption that actually does not apply to complex situations. Therefore, new, detailed modeling of anisotropic turbulence in three-

dimensional natural-convection flows with temperature stratification is necessary. This modeling requires a refined evaluation of the interaction between turbulence and buoyancy forces, which affect both incompressible fluids, because of hydrostatic force gradients, and compressible fluids, where density depends on temperature or concentration differences. The impact of buoyancy forces on production or dissipation of turbulence is represented in the k and ϵ equations by the term

$$G = -\rho \beta g_i \overline{u_i \phi} = \left(\frac{\partial \rho}{\partial T} \right)_p g_i \overline{u_i \phi}. \quad (2.1)$$

In Eq. 2.1,

$$\beta = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p \quad (2.2)$$

is the volumetric expansion coefficient and ϕ is the temperature fluctuation.

In the k - ϵ model, the buoyancy term G is usually approximated by

$$G \approx \beta \frac{\mu_t}{\sigma_t} g_i \frac{\partial T}{\partial x_i} = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p \frac{\mu_t}{\sigma_t} g_i \frac{\partial T}{\partial x_i}. \quad (2.3)$$

This approximation is rather crude, because it assumes that density variations depend only on temperature, and that the pressure field is in hydrostatic equilibrium. In fact, the influence of velocity fluctuations on the G term is neglected in Eq. 2.3. Whereas the first assumption is acceptable because it corresponds to the well-known Boussinesq approximation, the second is not, because the dynamic impact of coolant flow on buoyancy cannot be neglected in some situations. A more refined modeling of the G term is based on the so-called Hirt's assumption, which has been introduced into the COMMIX-2 code.⁵ It consists of setting

$$G = -\frac{1}{\rho^2} \frac{\mu_t}{\sigma_t} \frac{\partial \rho}{\partial x_i} \frac{\partial p}{\partial x_i}. \quad (2.4)$$

Equation 2.4 contains, as a subset, Eq. 2.3, which is obtained if the coolant density depends only on the temperature [$\rho = \rho(T)$],

$$\frac{\partial \rho}{\partial x_i} = \frac{\partial \rho}{\partial T} \frac{\partial T}{\partial x_i}, \quad (2.5)$$

and the pressure field is in hydrostatic equilibrium

$$\frac{\partial p}{\partial x_i} = \rho g_i. \quad (2.6)$$

It can easily be verified that Hirt's assumption implies the assumption that the scalar fluxes are given by

$$-\overline{u_i \phi} = \frac{1}{g_i \rho^2} \frac{\mu_t}{\sigma_t} \frac{\partial T}{\partial x_i} \frac{\partial p}{\partial x_i}. \quad (2.7)$$

If Eq. 2.6 holds, we obtain

$$-\overline{u_i \phi} = \frac{1}{\rho} \frac{\mu_t}{\sigma_t} \frac{\partial T}{\partial x_i}, \quad (2.8)$$

which corresponds to the assumption made in writing Eq. 2.3.

Numerical calculations made with the COMMIX-2 code⁵ proved, however, that even with Hirt's assumption, the performance of the k- ϵ model is poor in the case where fluid temperature is stratified. To cope with these problems, it is necessary, as a first step, to correctly compute the distribution of the turbulent fluxes $\overline{u_i \phi}$ by numerically solving three transport equations; these, in turn, contain a term that depends on temperature variance ϕ^2 , which is computed by solving a fourth transport equation.

The turbulence model based on the k- ϵ equations and on the four additional equations for $\overline{u_i \phi}$ and ϕ^2 was developed, as mentioned earlier, in the COMMIX-1C/ATM version of the code.³ Application of this variant to thermal stratification problems⁶ has shown substantial advantages with respect to the k- ϵ model used earlier. Although the discrepancy between experimental and computed results was reduced by approximately two-thirds with respect to earlier calculations, it became evident that further improvements required rigorous calculation of the Reynolds stresses, which appear in the transport equations for the scalar fluxes (see next section). Thus far, the Reynolds stresses had been approximated by algebraic expressions. Dropping the algebraic expressions and replacing them with six transport equations for $\overline{u_i u_j}$ implies adopting the RSM of turbulence. This model has been implemented in the new code variant CAPS-RSM. All of the mathematical and programming details of the RSM are documented in this report.

3 Model Equations for Scalar Fluxes and Variance of Temperature Fluctuations

3.1 Transport Equations for Scalar Fluxes

In this section, we present the transport equations for the scalar fluxes $\overline{u_i \phi}$ and their numerical treatment. After a literature review,⁷⁻¹⁰ we chose the following form of the transport equations for the scalar fluxes:

$$\begin{aligned} \frac{\partial}{\partial t}(\overline{u_i \phi}) + U_j \frac{\partial}{\partial x_j}(\overline{u_i \phi}) = & - \frac{\partial}{\partial x_i} \left(\overline{u_i u_j \phi} + \frac{1}{\rho} \overline{p \phi} \delta_{ij} \right) - \left(\overline{u_i u_j} \frac{\partial T}{\partial x_j} + \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} \right) \\ & - \beta g_i \overline{\phi^2} + \frac{1}{\rho} \overline{p} \frac{\partial \phi}{\partial x_i}. \end{aligned} \quad (3.1.1)$$

Equation 3.1.1 can be written in the more compact form

$$\frac{\partial(\overline{u_i\phi})}{\partial t} + U_j \frac{\partial(\overline{u_i\phi})}{\partial x_j} = \text{Diff} \overline{u_i\phi} + P_{i\phi} + G_{i\phi} + \pi_{i\phi}, \quad (3.1.2)$$

with the definitions

$$\text{Diff} \overline{u_i\phi} = -\frac{\partial}{\partial x_j} \left(\overline{u_i u_j \phi} + \frac{1}{\rho} \overline{p\phi} \delta_{ij} \right) \quad (\text{diffusive transport}), \quad (3.1.3)$$

$$P_{i\phi} = - \left(\overline{u_i u_j} \frac{\partial T}{\partial x_j} + \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} \right) \quad (\text{mean-field production}), \quad (3.1.4)$$

$$G_{i\phi} = - \beta g_i \overline{\phi^2} \quad (\text{buoyancy production}), \quad (3.1.5)$$

$$\pi_{i\phi} = \frac{1}{\rho} \overline{p} \frac{\partial \phi}{\partial x_i} \quad (\text{pressure-scalar gradient correlation}). \quad (3.1.6)$$

Diffusive transport is modeled as follows:

$$\begin{aligned} \text{Diff} \overline{u_i\phi} &= -\frac{\partial}{\partial x_j} \left(\overline{u_i u_j \phi} + \frac{1}{\rho} \overline{p\phi} \delta_{ij} \right) \\ &\simeq \frac{\partial}{\partial x_j} \left[\left(v_\ell + \frac{v_t}{\sigma_\phi} \right) \frac{\partial(\overline{u_i\phi})}{\partial x_j} \right] \\ &\simeq \frac{\partial}{\partial x_j} \left[\left(v_\ell + \frac{c_\mu k^2}{\sigma_\phi \varepsilon} \right) \frac{\partial(\overline{u_i\phi})}{\partial x_j} \right] \\ &\simeq \frac{\partial}{\partial x_j} \left[\left(v_\ell + c_{s\phi} \frac{k^2}{\varepsilon} \right) \frac{\partial(\overline{u_i\phi})}{\partial x_j} \right] \\ &\simeq \frac{\partial}{\partial x_j} \left[\Gamma_\phi^v \frac{\partial(\overline{u_i\phi})}{\partial x_j} \right], \end{aligned} \quad (3.1.7)$$

having used

$$v_t = c_\mu \frac{k^2}{\varepsilon}, \quad (3.1.8)$$

and defined

$$c_{s\phi} = \frac{c_\mu}{\sigma_\phi} \quad (3.1.9)$$

and

$$\Gamma_\phi^v = \nu_\ell + c_{s\phi} \frac{k^2}{\varepsilon}. \quad (3.1.10)$$

The Reynolds stresses $\overline{u_i u_j}$ that appear in the production and diffusive terms of Eq. 3.1.1 are computed by the respective transport equations, as explained in Sec. 4.1.

The pressure-scalar gradient correlation is modeled by

$$\pi_{i\phi} = \frac{1}{\rho} \overline{p \frac{\partial \phi}{\partial x_i}} = \pi_{i\phi}^1 + \pi_{i\phi}^2 + \pi_{i\phi}^3 + \pi_{i\phi}^w, \quad (3.1.11)$$

with

$$\pi_{i\phi}^1 = -c_{1\phi} \frac{\varepsilon}{k} \overline{u_i \phi} \quad (\text{turbulence contribution}), \quad (3.1.12a)$$

$$\pi_{i\phi}^2 = c_{2\phi} \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} \quad (\text{mean strain contribution}), \quad (3.1.12b)$$

$$\pi_{i\phi}^3 = c_{3\phi} \beta g_i \overline{\phi^2} = -c_{3\phi} G_{i\phi} \quad (\text{buoyancy contribution}), \quad (3.1.12c)$$

and

$$\pi_{i\phi}^w = -c_{1\phi} \frac{\varepsilon}{k} \overline{u_n \phi} \delta_{in} f\left(\frac{L}{x_n}\right) \quad (\text{wall effect}). \quad (3.1.12d)$$

Equation 3.1.12d represents the effect of the wall, n is the direction normal to the wall, and x_n is the distance from the wall. L is a suitable length scale, whereas the function $f(L/x_n)$ needs further specification. This topic will be dealt with further during the discussion of boundary conditions. In the computations, the function f has been chosen¹¹ so that its values approach unity close to the wall.

The values of the other constants used in the above equations have been determined experimentally,^{7,12} and are as follows:

$$\sigma_\phi = 1.3,$$

$$c_\mu = 0.09,$$

$$c_{s\phi} = c_\mu / \sigma_\phi = 0.09 / 1.3 (= 0.0692) \simeq 0.07,$$

$$c_{1\phi} = 3.1,$$

$$c_{2\phi} = 0.4,$$

$$c_{3\phi} = 0.5,$$

$$c_{1\phi} = 0.5.$$

Introducing Eqs. 3.1.3-3.1.12 into Eq. 3.1.1, we derive

$$\begin{aligned} \frac{\partial}{\partial t}(\overline{u_i\phi}) + U_j \frac{\partial}{\partial x_j}(\overline{u_i\phi}) &= \frac{\partial}{\partial x_j} \left[\Gamma_\phi^v \frac{\partial(\overline{u_i\phi})}{\partial x_j} \right] + P_{i\phi} + G_{i\phi}(1 - c_{3\phi}) \\ &\quad - c_{1\phi} \frac{\varepsilon}{k} \overline{u_i\phi} + c_{2\phi} \overline{u_j\phi} \frac{\partial U_i}{\partial x_j} + \pi_{i\phi}^w. \end{aligned} \quad (3.1.13)$$

If we use the identity

$$\nabla \cdot [\bar{U}(\overline{u_i\phi})] = \overline{u_i\phi}(\nabla \cdot \bar{U}) + \bar{U} \cdot \nabla(\overline{u_i\phi}), \quad (3.1.14)$$

and assume that the flow is free of divergence ($\nabla \cdot \bar{U} = 0$), the second term on the left-hand side of Eq. 3.1.13 can be written as

$$U_j \frac{\partial}{\partial x_j}(\overline{u_i\phi}) = \frac{\partial}{\partial x_j} [U_j(\overline{u_i\phi})]. \quad (3.1.15)$$

Introducing Eq. 3.1.15 into Eq. 3.1.13, we obtain

$$\begin{aligned} \frac{\partial(\overline{u_i\phi})}{\partial t} + \frac{\partial}{\partial x_j} \left[U_j(\overline{u_i\phi}) - \Gamma_\phi^v \frac{\partial(\overline{u_i\phi})}{\partial x_j} \right] &= P_{i\phi} + G_{i\phi}(1 - c_{3\phi}) \\ &\quad - c_{1\phi} \frac{\varepsilon}{k} \overline{u_i\phi} + c_{2\phi} \overline{u_j\phi} \frac{\partial U_i}{\partial x_j} + \pi_{i\phi}^w. \end{aligned} \quad (3.1.16)$$

Let us define the convective and diffusive fluxes as

$$J_{\phi ji}^c = U_j(\overline{u_i\phi}) \quad (3.1.17)$$

and

$$J_{\phi ji}^d = - \Gamma_\phi^v \frac{\partial(\overline{u_i\phi})}{\partial x_j}, \quad (3.1.18)$$

and the total (convective plus diffusive) flux as

$$\tilde{J}_{\phi ji} = J_{\phi ji}^c + J_{\phi ji}^d = U_j(\overline{u_i \phi}) - \Gamma_\phi^v \frac{\partial(\overline{u_i \phi})}{\partial x_j}. \quad (3.1.19)$$

Furthermore, let us define the source term as

$$S_{\phi i} = P_{i\phi} + G_{i\phi}(1 - c_{3\phi}) - c_{1\phi} \frac{\varepsilon}{k} \overline{u_i \phi} + c_{2\phi} \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} + \pi_{i\phi}^w. \quad (3.1.20)$$

With these definitions, we can write Eq. 3.1.16 in the compact form

$$\frac{\partial(\overline{u_i \phi})}{\partial t} + \frac{\partial}{\partial x_j} \tilde{J}_{\phi ji} = S_{\phi i}. \quad (3.1.21)$$

Let us denote the scalar transported quantity as

$$\Phi = \overline{u_i \phi}, \quad (3.1.22)$$

and drop superscripts and subscripts when no ambiguity exists. Thus, Eq. 3.1.21 can be written in the generalized form of the transport equation for the scalar Φ ,

$$\frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x_j} \tilde{J}_{\phi j} = S_\phi. \quad (3.1.23)$$

Multiplying Eq. 3.1.23 by ρ , and using the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho U_j)}{\partial x_j} = 0, \quad (3.1.24)$$

we obtain

$$\frac{\partial(\rho \Phi)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j \Phi) + \rho \Phi \frac{\partial U_j}{\partial x_j} - \rho \frac{\partial}{\partial x_j} \left(\Gamma_\phi^v \frac{\partial \Phi}{\partial x_j} \right) = \rho S_\phi. \quad (3.1.25)$$

As assumed earlier, $\partial U_j / \partial x_j \approx 0$; thus, we rewrite Eq. 3.1.25 as

$$\frac{\partial(\rho \Phi)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j \Phi) - \frac{\partial}{\partial x_j} \left(\rho \Gamma_\phi^v \frac{\partial \Phi}{\partial x_j} \right) = \rho S_\phi, \quad (3.1.26)$$

or

$$\frac{\partial}{\partial t} (\rho \Phi) + \frac{\partial}{\partial x_j} J_{\phi j} = \rho S_\phi, \quad (3.1.27)$$

with

$$J_{\phi j} = \rho \tilde{J}_{\phi j} = \rho U_j \Phi - \rho \Gamma_{\phi}^v \frac{\partial \Phi}{\partial x_j} = \rho U_j \Phi - \Gamma_{\phi} \frac{\partial \Phi}{\partial x_j}, \quad (3.1.28)$$

and

$$\Gamma_{\phi} = \rho \Gamma_{\phi}^v = \mu_{\ell} + c_{s\phi} \rho \frac{k^2}{\varepsilon}. \quad (3.1.29)$$

If we integrate Eq. 3.1.27 over the volume V_f of the fluid in a cell, we obtain

$$\int_{V_f} \frac{\partial(\rho\Phi)}{\partial t} dV + \int_{V_f} \left(\frac{\partial}{\partial x_j} J_{\phi j} \right) dV = \int_{V_f} \rho S_{\phi} dV. \quad (3.1.30)$$

Using the Gauss theorem, we replace the volume integral of the divergence of vector J with the fluxes through the boundary surfaces. By indexing the center node of a cell with (i,j,k) , we have

$$\begin{aligned} \int_{V_f} \frac{\partial(\rho\Phi)}{\partial t} dV + \int_{A_{f,i+1/2}} J_{\phi i} dA - \int_{A_{f,i-1/2}} J_{\phi i} dA + \int_{A_{f,j+1/2}} J_{\phi j} dA - \int_{A_{f,j-1/2}} J_{\phi j} dA \\ + \int_{A_{f,k+1/2}} J_{\phi k} dA - \int_{A_{f,k-1/2}} J_{\phi k} dA = \int_{V_f} \rho S_{\phi} dV. \end{aligned} \quad (3.1.31)$$

In this equation, $A_{f,i\pm 1/2}$, $A_{f,j\pm 1/2}$, and $A_{f,k\pm 1/2}$ are the cross flow areas of the surfaces that bound the cell in the x , y , and z directions, respectively. Denoting with the symbols $\langle \rangle$ and $\langle \rangle_3$ mean values over surfaces and volumes, respectively, Eq. 3.1.31 is discretized as follows:

$$\begin{aligned} \frac{V_f}{\Delta t} [(\rho\Phi)^{n+1} - (\rho\Phi)^n]_{ijk} + \langle J_{\phi}^c A_f \rangle_{i+1/2,j,k}^{n+1} - \langle J_{\phi}^c A_f \rangle_{i-1/2,j,k}^{n+1} + \langle J_{\phi}^c A_f \rangle_{i,j+1/2,k}^{n+1} \\ - \langle J_{\phi}^c A_f \rangle_{i,j-1/2,k}^{n+1} + \langle J_{\phi}^c A_f \rangle_{i,j,k+1/2}^{n+1} - \langle J_{\phi}^c A_f \rangle_{i,j,k-1/2}^{n+1} \\ + A_{f,i+1/2} \left\langle \Gamma_{\phi} \frac{\partial \Phi}{\partial x} \right\rangle_{i+1/2,j,k}^{n+1} - A_{f,i-1/2} \left\langle \Gamma_{\phi} \frac{\partial \Phi}{\partial x} \right\rangle_{i-1/2,j,k}^{n+1} + A_{f,j+1/2} \left\langle \Gamma_{\phi} \frac{\partial \Phi}{\partial y} \right\rangle_{i,j+1/2,k}^{n+1} \\ - A_{f,j-1/2} \left\langle \Gamma_{\phi} \frac{\partial \Phi}{\partial y} \right\rangle_{i,j-1/2,k}^{n+1} + A_{f,k+1/2} \left\langle \Gamma_{\phi} \frac{\partial \Phi}{\partial z} \right\rangle_{i,j,k+1/2}^{n+1} - A_{f,k-1/2} \left\langle \Gamma_{\phi} \frac{\partial \Phi}{\partial z} \right\rangle_{i,j,k-1/2}^{n+1} \\ = V_f \langle \rho S_{\phi} \rangle_3. \end{aligned} \quad (3.1.32)$$

In Eq. 3.1.32, we separate the convective terms, represented by the vector J^c , from the diffusive terms. The convective terms are computed as follows:

$$\begin{aligned}
\langle J_\phi^c A_f \rangle_{\alpha+1/2}^{n+1} &= \langle \rho U \Phi A_f \rangle_{\alpha+1/2}^{n+1} = \langle F \Phi \rangle_{\alpha+1/2}^{n+1} \\
&= [0, F_{\alpha+1/2}] \Phi_\alpha^{n+1} - [0, -F_{\alpha+1/2}] \Phi_{\alpha+1}^{n+1},
\end{aligned} \tag{3.1.33a}$$

$$\langle J_\phi^c A_f \rangle_{\alpha-1/2}^{n+1} = [0, F_{\alpha-1/2}] \Phi_{\alpha-1}^{n+1} - [0, -F_{\alpha-1/2}] \Phi_\alpha^{n+1}, \tag{3.1.33b}$$

with

$$F_{\alpha\pm 1/2} = (\rho U A)_{\alpha\pm 1/2} \quad (\alpha = i, j, k). \tag{3.1.34}$$

In Eqs. 3.1.33a and b, the symbol [a,b] denotes the maximum of two real numbers a and b.

The diffusive terms are computed by

$$A_{f_{\alpha+1/2}} \left\langle \Gamma_\phi \frac{\partial \Phi}{\partial x_\alpha} \right\rangle_{\alpha+1/2}^{n+1} = \frac{A_{f_{\alpha+1/2}} (\Phi_{\alpha+1} - \Phi_\alpha)^{n+1}}{\frac{1}{2} \left(\frac{\Delta x_\alpha}{\Gamma_{\phi, \alpha}} + \frac{\Delta x_{\alpha+1}}{\Gamma_{\phi, \alpha+1}} \right)} = D_{\alpha+1/2}^{\Phi, n+1} (\Phi_{\alpha+1} - \Phi_\alpha)^{n+1}, \tag{3.1.35a}$$

$$A_{f_{\alpha-1/2}} \left\langle \Gamma_\phi \frac{\partial \Phi}{\partial x_\alpha} \right\rangle_{\alpha-1/2}^{n+1} = \frac{A_{f_{\alpha-1/2}} (\Phi_\alpha - \Phi_{\alpha-1})^{n+1}}{\frac{1}{2} \left(\frac{\Delta x_{\alpha-1}}{\Gamma_{\phi, \alpha-1}} + \frac{\Delta x_\alpha}{\Gamma_{\phi, \alpha}} \right)} = D_{\alpha-1/2}^{\Phi, n+1} (\Phi_\alpha - \Phi_{\alpha-1})^{n+1}, \tag{3.1.35b}$$

$$(\alpha = i, j, k),$$

with the definitions

$$D_{\alpha+1/2}^\Phi = \frac{A_{f_{\alpha+1/2}}}{\frac{1}{2} \left(\frac{\Delta x_\alpha}{\Gamma_{\phi, \alpha}} + \frac{\Delta x_{\alpha+1}}{\Gamma_{\phi, \alpha+1}} \right)} \tag{3.1.36a}$$

and

$$D_{\alpha-1/2}^\Phi = \frac{A_{f_{\alpha-1/2}}}{\frac{1}{2} \left(\frac{\Delta x_{\alpha-1}}{\Gamma_{\phi, \alpha-1}} + \frac{\Delta x_\alpha}{\Gamma_{\phi, \alpha}} \right)}. \tag{3.1.36b}$$

Introducing Eqs. 3.1.33–3.1.35 into Eq. 3.1.32, we derive, after rearranging,

$$\begin{aligned}
& \Phi_{i,j,k}^{n+1} \left\{ \frac{(V_f \rho^{n+1})_{i,j,k}}{\Delta t} + [0, F_{i+1/2}] + [0, F_{j+1/2}] + [0, F_{k+1/2}] + [0, -F_{i-1/2}] \right. \\
& \quad \left. + [0, -F_{j-1/2}] + [0, -F_{k-1/2}] + D_{i+1/2}^\Phi + D_{i-1/2}^\Phi + D_{j+1/2}^\Phi + D_{j-1/2}^\Phi + D_{k+1/2}^\Phi + D_{k-1/2}^\Phi \right\} \\
& - \Phi_{i+1}^{n+1} \{ [0, -F_{i+1/2}] + D_{i+1/2}^\Phi \} - \Phi_{i-1}^{n+1} \{ [0, F_{i-1/2}] + D_{i-1/2}^\Phi \} \\
& - \Phi_{j+1}^{n+1} \{ [0, -F_{j+1/2}] + D_{j+1/2}^\Phi \} - \Phi_{j-1}^{n+1} \{ [0, F_{j-1/2}] + D_{j-1/2}^\Phi \} \\
& - \Phi_{k+1}^{n+1} \{ [0, -F_{k+1/2}] + D_{k+1/2}^\Phi \} - \Phi_{k-1}^{n+1} \{ [0, F_{k-1/2}] + D_{k-1/2}^\Phi \} \\
& = V_{f,i,j,k} \frac{(\rho \Phi)_{i,j,k}^n}{\Delta t} + (V_f \rho)_{i,j,k}^n \langle S_\Phi \rangle_3^{n+1}.
\end{aligned} \tag{3.1.37}$$

Let us introduce the usual convention of indexing with

- 0 for i, j, k
- 1 for $i-1, j, k$
- 2 for $i+1, j, k$
- 3 for $i, j-1, k$
- 4 for $i, j+1, k$
- 5 for $i, j, k-1$
- 6 for $i, j, k+1$.

Equation 3.1.33 can be written in the compact form

$$a_0^\Phi \Phi_0^{n+1} - \sum_{\beta=1}^6 a_\beta^\Phi \Phi_\beta^{n+1} = b_0^\Phi, \tag{3.1.38}$$

with the definition of coefficients

$$\begin{aligned}
a_0^\Phi &= \frac{V_{f0} \rho_0^{n+1}}{\Delta t} + [0, F_{i+1/2}] + [0, F_{j+1/2}] + [0, F_{k+1/2}] \\
&\quad + [0, -F_{i-1/2}] + [0, -F_{j-1/2}] + [0, -F_{k-1/2}] \\
&\quad + D_{i+1/2}^\Phi + D_{i-1/2}^\Phi + D_{j+1/2}^\Phi + D_{j-1/2}^\Phi + D_{k+1/2}^\Phi + D_{k-1/2}^\Phi
\end{aligned} \tag{3.1.39a}$$

$$a_1^\Phi = [0, F_{i-1/2}] + D_{i-1/2}^\Phi \tag{3.1.39b}$$

$$a_2^\Phi = [0, -F_{i+1/2}] + D_{i+1/2}^\Phi \tag{3.1.39c}$$

$$a_3^\Phi = [0, F_{j-1/2}] + D_{j-1/2}^\Phi \quad (3.1.39d)$$

$$a_4^\Phi = [0, -F_{j+1/2}] + D_{j+1/2}^\Phi \quad (3.1.39e)$$

$$a_5^\Phi = [0, F_{k-1/2}] + D_{k-1/2}^\Phi \quad (3.1.39f)$$

$$a_6^\Phi = [0, -F_{k+1/2}] + D_{k+1/2}^\Phi \quad (3.1.39g)$$

$$b_0^\Phi = V_{f_0} \frac{(\rho\Phi)_0^n}{\Delta t} + V_{f_0} \rho_0^{n+1} \langle S_\Phi \rangle_3^{n+1}. \quad (3.1.39h)$$

By recalling the definitions of $S_{\Phi i}$ (Eq. 3.1.20), $P_{i\Phi}$ (Eq. 3.1.4), and $G_{i\Phi}$ (Eq. 3.1.5), we can write the right-hand side of Eq. 3.1.38 in detail as

$$\begin{aligned} b_0^\Phi &= b_0^{\overline{u_i\Phi}} = V_{f_0} \frac{(\overline{\rho u_i\Phi})_0^n}{\Delta t} + V_{f_0} \rho_0^{n+1} \left\langle \rho_{i\Phi} + G_{i\Phi}(1 - c_{3\Phi}) - c_{1\Phi} \frac{\varepsilon}{k} \overline{u_i\Phi} + c_{2\Phi} \frac{\varepsilon}{k} \overline{u_j\Phi} \frac{\partial U_i}{\partial x_j} + \pi_{i\Phi}^w \right\rangle_3^{n+1} \\ &= V_{f_0} \frac{(\overline{\rho u_i\Phi})_0^n}{\Delta t} + V_{f_0} \rho_0^{n+1} \left[- \left(\overline{u_i u_j} \frac{\partial T}{\partial x_j} + \overline{u_j\Phi} \frac{\partial U_i}{\partial x_j} \right) - \beta g_i \overline{\Phi^2} (1 - c_{3\Phi}) \right. \\ &\quad \left. - c_{1\Phi} \frac{\varepsilon}{k} \overline{u_i\Phi} + c_{2\Phi} \overline{u_j\Phi} \frac{\partial U_i}{\partial x_j} + \pi_{i\Phi}^w \right]^{n+1}, \end{aligned} \quad (3.1.40)$$

where we finally drop the symbol $\langle \rangle_3$.

Using the discretized form of the continuity equation (see Eq. 2.32 of Ref. 13)

$$\begin{aligned} V_{f_0} \frac{\rho_0^{n+1}}{\Delta t} &+ [0, F_{i+1/2}] - [0, -F_{i+1/2}] + [0, -F_{i-1/2}] - [0, F_{i-1/2}] \\ &+ [0, F_{j+1/2}] - [0, -F_{j+1/2}] + [0, -F_{j-1/2}] - [0, F_{j-1/2}] \\ &+ [0, F_{k+1/2}] - [0, -F_{k+1/2}] + [0, -F_{k-1/2}] - [0, F_{k-1/2}] = V_{f_0} \frac{\rho_0^n}{\Delta t}, \end{aligned} \quad (3.1.41)$$

we obtain the so-called second form of the coefficient a_0^Φ , i.e.,

$$\begin{aligned} a_0^{\Pi \overline{u_i\Phi}} &= \frac{V_{f_0} \rho_0^n}{\Delta t} + [0, F_{i-1/2}] + [0, -F_{i+1/2}] + [0, F_{j-1/2}] + [0, -F_{j+1/2}] \\ &+ [0, F_{k-1/2}] + [0, -F_{k+1/2}] \end{aligned}$$

$$+ D_{i+1/2} + D_{j+1/2} + D_{k+1/2} + D_{i-1/2} + D_{j-1/2} + D_{k-1/2}. \quad (3.1.42)$$

3.2 Transport Equation for Variance of Temperature Fluctuations

In this section, we present the transport equation for the scalar variance of temperature fluctuations $\bar{\phi}^2$ and its numerical treatment. After a literature review,⁷⁻¹⁰ we chose the following form of the transport equation for this scalar:

$$\frac{\partial \bar{\phi}^2}{\partial t} + U_j \frac{\partial \bar{\phi}^2}{\partial x_j} = - \frac{\partial}{\partial x_j} \left(\overline{u_j \phi^2} \right) + \frac{\partial}{\partial x_j} \left(\frac{\lambda}{\rho c_p} \frac{\partial \bar{\phi}^2}{\partial x_j} \right) - 2 \overline{u_j \phi} \frac{\partial T}{\partial x_j} - 2 \frac{\lambda}{\rho c_p} \frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_j}. \quad (3.2.1)$$

Equation 3.2.1 can be written in the more compact form

$$\frac{\partial \bar{\phi}^2}{\partial t} + U_j \frac{\partial \bar{\phi}^2}{\partial x_j} = D_t \bar{\phi}^2 + D_\ell \bar{\phi}^2 + P_\phi - \varepsilon_\phi, \quad (3.2.2)$$

where

$$D_t \bar{\phi}^2 = - \frac{\partial}{\partial x_j} \left(\overline{u_j \phi^2} \right) \equiv \frac{\partial}{\partial x_j} \left[c_\phi \frac{k^2}{\varepsilon} \frac{\partial \bar{\phi}^2}{\partial x_j} \right] \quad (\text{turbulent diffusion}), \quad (3.2.3)$$

$$D_\ell \bar{\phi}^2 = \frac{\partial}{\partial x_j} \left(\frac{\lambda}{\rho c_p} \frac{\partial \bar{\phi}^2}{\partial x_j} \right) \quad (\text{molecular diffusion}), \quad (3.2.4)$$

$$P_\phi = - 2 \overline{u_j \phi} \frac{\partial T}{\partial x_j} \quad (\text{mean-field production}), \quad (3.2.5)$$

and

$$\varepsilon_\phi = \frac{2\lambda}{\rho c_p} \frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_j} = \frac{\varepsilon}{k} \bar{\phi}^2 \quad (\text{dissipation of fluctuation}). \quad (3.2.6)$$

The values of the constants used in the above equations have been determined experimentally⁷ as $c_\phi = 0.13$ and $R = 0.5$.

By defining one-half of the variance of temperature fluctuation as

$$g = \frac{1}{2} \bar{\phi}^2, \quad (3.2.7)$$

the transport equation for scalar fluctuation, referred to as the "g equation," can be reformulated as

$$\frac{\partial g}{\partial t} + \frac{\partial(U_j g)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(c_\phi \frac{k^2}{\epsilon} \frac{\partial g}{\partial x_j} + \frac{\lambda}{\rho c_p} \frac{\partial g}{\partial x_j} \right) - \overline{u_j \phi} \frac{\partial T}{\partial x_j} - \frac{\epsilon}{k} \frac{g}{R}. \quad (3.2.8)$$

By defining

$$\Gamma_g = \Gamma_{gt} + \Gamma_{g\ell} = c_\phi \frac{k^2}{\epsilon} + \frac{\lambda}{\rho c_p}, \quad (3.2.9)$$

$$P_g = \frac{1}{2} P_\phi = - \overline{u_j \phi} \frac{\partial T}{\partial x_j}, \quad (3.2.10)$$

and

$$\epsilon_g = \frac{1}{2} \epsilon_\phi = \frac{\epsilon}{k} \frac{g}{R}, \quad (3.2.11)$$

Eq. 3.2.8 can be abbreviated to

$$\frac{\partial g}{\partial t} + \frac{\partial(U_j g)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\Gamma_g \frac{\partial g}{\partial x_j} \right) + P_g - \epsilon_g. \quad (3.2.12)$$

Let us define the convective and diffusive fluxes of the variance of temperature fluctuations by

$$J_{gj}^c = U_j g \quad (3.2.13)$$

and

$$J_{gj}^d = -\Gamma_g \frac{\partial g}{\partial x_j}, \quad (3.2.14)$$

and the total (convective plus diffusive) flux by

$$J_{gj} = J_{gj}^c + J_{gj}^d = U_j g - \Gamma_g \frac{\partial g}{\partial x_j}. \quad (3.2.15)$$

Furthermore, let us define the source term as

$$S_g = P_g - \epsilon_g. \quad (3.2.16)$$

With these definitions, Eq. 3.2.12 can be written in compact form as

$$\frac{\partial g}{\partial t} + \frac{\partial(J_{gj})}{\partial x_j} = S_g. \quad (3.2.17)$$

If we use the procedure that was followed for the scalar fluxes, we transform the differential equation Eq. 3.2.17 into the linear algebraic equation

$$a_0^g g_0^{n+1} - \sum_{\beta=1}^6 a_{\beta}^g g_{\beta}^{n+1} = b_0^g, \quad (3.2.18)$$

with the same expressions for coefficients a_0^g and a_{β}^g as coefficients a_0^{ϕ} and a_{β}^{ϕ} (Eqs. 3.1.39a-3.1.39g). The expression for b_0^g is given by

$$\begin{aligned} b_0^g &= b_0^{1/2} = \frac{V_{f0}(\rho g)_0^n}{\Delta t} + V_{f0} \rho_0^{n+1} \langle S_g \rangle_3^{n+1} \\ &= \frac{V_{f0}(\rho g)_0^n}{\Delta t} + V_{f0} \rho_0^{n+1} \left[\overline{u_j \phi} \frac{\partial T}{\partial x_j} - \left(\frac{\varepsilon}{k} \right)^{n+1} \frac{g^{n+1}}{R} \right]. \end{aligned} \quad (3.2.19)$$

3.3 Boundary Conditions

In the immediate vicinity of a solid wall, there is a large variation in the values of turbulence properties. Therefore, to predict the correct values of momentum flux, energy flux, and the gradients of turbulence parameters such as $\overline{u_i \phi}$, $\phi^2/2$, ε , and $\overline{u_i u_j}$, the COMMIX-1C/RSM code applies a special treatment called the wall function treatment.

Figures 1 and 2 show the two-layer wall function model used in COMMIX-1C/RSM, where P is the node adjacent to the wall, y_p is the distance from P to the wall, and y_{ℓ} is the thickness of the viscous sublayer. The distance y_p is fixed, depending on the mesh system. The thickness of the viscous sublayer y_{ℓ} , however, is not a constant and must be computed. It is evaluated by matching the velocity at the edge of the viscous sublayer to the value obtained from the law of the wall (see Ref. 3 for details).

Figure 1. Two-layer wall function model where $y_p > y_{\ell}$

Figure 2. Two-layer wall function model where $y_p \leq y_\ell$

3.3.1 Boundary Conditions for Scalar Fluxes

Case $y_p < y_\ell$

If, with reference to Figs. 1 and 2, $y_p < y_\ell$ (hence, the first mesh node adjacent to the wall is in the laminar sublayer), we use the boundary conditions

$$(\overline{u_i \phi})_P = c_\mu \frac{k^2}{\varepsilon} \frac{\partial T}{\partial x_i} \quad (i = 1, 2, 3), \quad (3.3.1.1)$$

suggested by Ref. 14.

Case $y_p > y_\ell$

If $y_p > y_\ell$ (hence, the mesh node adjacent to the wall is in the turbulent region), a boundary condition for the scalar fluxes $\overline{u_i \phi}$ can be obtained from the average conservation equation for the fluid temperature⁷

$$\frac{\partial T}{\partial t} + U_i \frac{\partial T}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\lambda}{\rho c_p} \frac{\partial T}{\partial x_i} - \overline{u_i \phi} \right) + S_\phi. \quad (3.3.1.2)$$

In a steady-state situation and under the assumption of negligible contributions from convective and source terms, we have

$$-\overline{u_i \phi} = -\frac{\lambda}{\rho c_p} \frac{\partial T}{\partial x_i} = -\frac{\mu_t}{\rho \sigma_t} \frac{\partial T}{\partial x_i}, \quad (3.3.1.3)$$

having used the following definition of the turbulence Prandtl number for heat transport:

$$\sigma_t = \frac{v_t}{\lambda} \rho c_p = \frac{\mu_t c_p}{\lambda}. \quad (3.3.1.4)$$

We use $\sigma_t = 0.9$. Equation 3.3.1.3 is used for every coordinate direction, i.e., for each of the three scalar components of the transport equations for heat fluxes. In the particular case of the coordinate direction perpendicular to the wall, say the y direction, Eq. 3.3.1.3 implies

$$-\overline{u_i \phi} \begin{cases} = 0 & \text{for unheated wall,} \\ = \frac{q_w}{\rho c_p} & \text{for heated wall,} \end{cases} \quad (3.3.1.5)$$

with

$$q_w = -\lambda \left(\frac{\partial T}{\partial y} \right)_w. \quad (3.3.1.6)$$

By using the wall temperature function,¹⁵

$$-T^+ = \frac{T_w - T_p}{T^*} = \frac{\sigma_t}{K} \ln y^+ + \text{a constant}, \quad (3.3.1.7)$$

with

$$T^* = \frac{q_w}{\rho c_p u^*} \quad (3.3.1.8)$$

and

$$y^+ = \frac{y u^*}{\nu}, \quad (3.3.1.9)$$

where T_p denotes the fluid temperature at node P and the boundary condition (Eq. 3.3.1.5) can be expressed in terms of the auxiliary temperature T^* (defined by Eq. 3.3.1.8) and of the friction velocity.

Letting $T = T_p - T_w$ (hence, $T^+ = T/T^*$), and differentiating, we obtain

$$-\frac{dT}{dy} = T^* \frac{\sigma_t}{Ky}. \quad (3.3.1.10)$$

Using

$$u^* = \frac{v_t}{Ky}, \quad (3.3.1.11)$$

we derive

$$-\overline{u_1\phi} = \frac{q_w}{\rho c_p} = -\frac{\lambda}{\rho c_p} \frac{dT}{dy} = \frac{T^* \sigma_t}{Ky} \frac{\lambda}{\rho c_p} = \frac{T^* v_t}{Ky} = T^* u^*. \quad (3.3.1.12)$$

3.3.2 Boundary Conditions for Variance of Temperature Fluctuations

Case $y_p < y_\ell$

Denoting y the coordinate direction normal to the wall, and taking into account only contributions in the y direction, the steady-state equation for the variance of temperature fluctuations can be written as

$$\frac{\partial}{\partial y}(vg) = \frac{\partial}{\partial y} \left(\Gamma_g \frac{\partial g}{\partial y} \right) - \overline{v\phi} \frac{\partial T}{\partial y} - \frac{\varepsilon}{k} \frac{g}{R}. \quad (3.3.2.1)$$

Integrating this equation over the thickness of the laminar sublayer, we obtain

$$\int_0^{y_\ell} \frac{\partial}{\partial y}(vg) dy = \int_0^{y_\ell} \frac{\partial}{\partial y} \left(\Gamma_g \frac{\partial g}{\partial y} \right) dy - \int_0^{y_\ell} \overline{v\phi} \frac{\partial T}{\partial y} dy - \frac{1}{R} \int_0^{y_\ell} \frac{\varepsilon}{k} g dy; \quad (3.3.2.2)$$

hence, letting $vg = 0$ at the wall,

$$\begin{array}{cccccc} (vg)_{y_\ell} & = & \left(\Gamma_g \frac{\partial g}{\partial y} \right)_{y_\ell} & - & \left(\Gamma_g \frac{\partial g}{\partial y} \right)_w & - & \int_0^{y_\ell} \overline{v\phi} \frac{\partial T}{\partial y} dy & - & \frac{1}{R} \int_0^{y_\ell} \frac{\varepsilon}{k} g dy. \\ \text{Term 1} & & 2 & & 3 & & 4 & & 5 \end{array} \quad (3.3.2.3)$$

The terms in Eq. 3.3.2.3 are evaluated as follows:

$$\text{Term 1} = (vg)_{y_\ell} \approx (vg)_p \frac{y_\ell}{y_p}, \quad (3.3.2.4)$$

$$\text{Term 2} = \left(\Gamma_g \frac{\partial g}{\partial y} \right)_{y_\ell} \approx \Gamma_{g_\ell} \frac{g_\ell - g_p}{y_\ell - y_p}, \quad (3.3.2.5)$$

$$\text{Term 3} = \left(\Gamma_g \frac{\partial g}{\partial y} \right)_w \approx \Gamma_{g_p} \frac{g_p - g_w}{y_p}, \quad (3.3.2.6)$$

$$\text{Term 4} = \int_0^{y_\ell} (\overline{v\phi}) \frac{\partial T}{\partial y} dy = (\overline{v\phi})_{y_\ell/2} \int_0^{y_\ell} \frac{\partial T}{\partial y} dy = \frac{u^* T^*}{2} \int_0^{y_\ell} \frac{\partial T}{\partial y} dy. \quad (3.3.2.7)$$

Term 5 is evaluated below.

Using Eqs. 3.3.1.12 and 3.3.1.4, we obtain

$$-\frac{dT}{dy} = \frac{\rho c_p}{\lambda} u^* T^* = \frac{\sigma_t}{v_t} u^* T^*. \quad (3.3.2.8)$$

Introducing Eq. 3.3.2.8 into Eq. 3.3.2.7, we derive

$$\text{Term 4} \approx -\frac{u^* T^*}{2} \frac{u^* T^* \sigma_t}{v_t} y_\ell = -\frac{(u^* T^*)^2 \sigma_t}{2v_t} y_\ell. \quad (3.3.2.9)$$

Term 5 is evaluated by using, in the laminar sublayer,¹⁶

$$k^+ = \frac{k}{u^{*2}} = A^+ y^{+2} = A^+ \left(\frac{yu^*}{v_\ell} \right)^2 \quad A^+ \approx 0.025 \quad (3.3.2.10)$$

$$\varepsilon^+ = \frac{\varepsilon v_\ell}{u^{*4}} = 2A^+ \quad (3.3.2.11)$$

$$\frac{\varepsilon}{k} = \frac{2v_\ell}{y^2}. \quad (3.3.2.12)$$

Hence,

$$\text{Term 5} = -\frac{1}{R} \int_0^{y_\ell} \frac{\varepsilon}{k} g dy = -\frac{1}{R} \int_0^{y_\ell} \frac{2v_\ell}{y^2} g dy. \quad (3.3.2.13)$$

Analogous with the definition $T^+ = T/T^*$ and with the linear distribution

$$T^+ = \text{Pr } y^+, \quad (3.3.2.14)$$

we assume that

$$\phi^+ = \frac{\phi}{T^*} = c_g y^+; \quad (3.3.2.15)$$

hence,

$$g^+ = \frac{1}{2} \phi^{+2} = \frac{1}{2} \frac{\phi^2}{T^{*2}} = \frac{1}{2} c_g^2 y^{+2} \quad (3.3.2.16)$$

and

$$g = \frac{1}{2} \phi^2 = \frac{1}{2} c_g^2 T^{*2} y^{+2} = \frac{1}{2} c_g^2 T^{*2} \left(\frac{yu^*}{v_\ell} \right)^2. \quad (3.3.2.17)$$

If we introduce Eq. 3.3.2.13, we have

$$\text{Term 5} = -\frac{2v_\ell}{R} \int_0^{y_\ell} \frac{g}{y^2} dy = -\frac{2v_\ell}{R} c_g^2 \int_0^{y_\ell} \frac{T^* u^*}{2 v_\ell^2} dy = -\frac{c_g^2}{R v_\ell} (T^* u^*)^2 y_\ell. \quad (3.3.2.18)$$

When all of the terms are assembled, Eq. 3.3.2.3 yields

$$\begin{aligned} & g_p \left(v_p \frac{y_\ell}{y_p} + \frac{\Gamma_{gl}}{y_\ell - y_p} + \frac{\Gamma_{gp}}{y_p} \right) \\ &= \Gamma_{gl} \frac{g_\ell}{y_\ell - y_p} + \Gamma_{gp} \frac{g_w}{y_p} + \frac{(u^* T^*)^2 \sigma_t}{2v_t} y_\ell - \frac{c_g^2}{R v_\ell} (u^* T^*)^2 y_\ell, \end{aligned} \quad (3.3.2.19)$$

from which we obtain g_p . For lack of specific information, we assumed that $c_g = 1$.

Case $y_p > y_\ell$

In the case when the node P lies in the turbulent region, a boundary condition can be obtained by assuming equilibrium between production and dissipation of the variance of temperature fluctuations. Hence,

$$P_\phi = -2\overline{v\phi} \left(\frac{\partial T}{\partial y} \right)_w = \frac{\varepsilon}{k} \frac{2g_w}{R} = \varepsilon_\phi \quad (3.3.2.20)$$

and

$$\left(\frac{\partial T}{\partial y} \right)_w = -\frac{\varepsilon}{k} \frac{g_w}{R(\overline{v\phi})}. \quad (3.3.2.21)$$

Relating the scalar flux $\overline{v\phi}$ to the temperature gradient, and using Eq. 3.3.2.21, we have

$$-\overline{v\phi} = \frac{v_t}{\sigma_t} \left(\frac{\partial T}{\partial y} \right)_w = -\frac{v_t}{\sigma_t} \frac{\varepsilon}{k} \frac{g_w}{R(\overline{v\phi})}; \quad (3.3.2.22)$$

hence,

$$\begin{aligned} g_w &= (\overline{v\phi})^2 \frac{\sigma_t k R}{v_t \varepsilon} \\ &= (\overline{v\phi})^2 \sigma_t \frac{k R}{\varepsilon} \frac{\varepsilon}{c_\mu k^2} = (\overline{v\phi})^2 \frac{\sigma_t R}{c_\mu k} \\ &= \frac{(u^* T^*)^2 R \sigma_t}{c_\mu k}. \end{aligned} \quad (3.3.2.23)$$

Using

$$k = k_w = \frac{u^{*2}}{\sqrt{c_\mu}} \quad (3.3.2.24)$$

and

$$T^* u^* = q_w / \rho c_p, \quad (3.3.2.25)$$

we obtain

$$g_w = \left(\frac{q_w}{\rho c_p} \right)^2 \frac{R \sigma_t}{c_\mu \frac{u^{*2}}{\sqrt{c_\mu}}} = \left(\frac{q_w}{\rho c_p u^*} \right)^2 \frac{R \sigma_t}{\sqrt{c_\mu}}. \quad (3.3.2.26)$$

An alternative formulation is

$$g_w = \frac{T^{*2} R \sigma_t}{\sqrt{c_\mu}}. \quad (3.3.2.27)$$

4 Reynolds Stress Model

4.1 Transport Equations for Reynolds Stresses

4.1.1 Modeling of Transport Equations

The transport equations for the Reynolds stresses have been derived by Chou¹⁷ in the form

$$\frac{\partial \overline{u_i u_j}}{\partial t} + U_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} = - \frac{\partial}{\partial x_\ell} (\overline{u_\ell u_i u_j}) - \frac{1}{\rho} \left(\frac{\partial \overline{u_j p}}{\partial x_i} + \frac{\partial \overline{u_i p}}{\partial x_j} \right) + P_{ij} + G_{ij} + \pi_{ij} - \epsilon_{ij}, \quad (4.1.1.1)$$

with

$$P_{ij} = - \overline{u_i u_\ell} \frac{\partial U_j}{\partial x_\ell} - \overline{u_j u_\ell} \frac{\partial U_i}{\partial x_\ell}, \quad (4.1.1.2)$$

$$G_{ij} = - \beta g_i \overline{u_j \phi} - \beta g_j \overline{u_i \phi}, \quad (4.1.1.3)$$

$$\pi_{ij} = \frac{p}{\rho} \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right), \quad (4.1.1.4)$$

$$\varepsilon_{ij} = 2\nu \frac{\partial u_i}{\partial x_\ell} \frac{\partial u_j}{\partial x_\ell}. \quad (4.1.1.5)$$

The first two terms at the right-hand side of Eq. 4.1.1.1 are diffusion terms; the first depends only on velocity fluctuation, the second on pressure and velocity correlations. P_{ij} is the stress production due to the mean flow; G_{ij} , the stress production due to buoyancy forces; π_{ij} , the pressure strain tensor, and ε_{ij} , the viscous dissipation tensor.

The diffusion terms are modeled by a gradient law as

$$\begin{aligned} \text{Diff}(\overline{u_i u_j}) &= -\frac{\partial}{\partial x_\ell} (\overline{u_\ell u_i u_j}) - \frac{1}{\rho} \left(\frac{\partial \overline{u_j p}}{\partial x_i} + \frac{\partial \overline{u_i p}}{\partial x_j} \right) \\ &\approx \frac{\partial}{\partial x_\ell} \left[\nu_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} + c_s \frac{\partial}{\partial x_\ell} \left(\frac{k}{\varepsilon} \overline{u_k u_\ell} \frac{\partial \overline{u_i u_j}}{\partial x_k} \right) \right] \\ &\approx \frac{\partial}{\partial x_\ell} \left(\nu_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} + c_s \frac{k^2}{\varepsilon} \frac{\partial \overline{u_i u_j}}{\partial x_\ell} \right). \end{aligned} \quad (4.1.1.6)$$

The pressure strain tensor is modeled as the sum of four contributions by

$$\pi_{ij} = \frac{p}{\rho} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \approx \pi_{ij}^1 + \pi_{ij}^2 + \pi_{ij}^3 + \pi_{ij}^w, \quad (4.1.1.7)$$

with

$$\pi_{ij}^1 = -c_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) = -c_1 \varepsilon a_{ij}, \quad (4.1.1.8)$$

$$\pi_{ij}^2 = -c_2 \left(P_{ij} - \frac{2}{3} P \delta_{ij} \right), \quad (4.1.1.9)$$

$$\pi_{ij}^3 = -c_3 \left(G_{ij} - \frac{2}{3} G \delta_{ij} \right), \quad (4.1.1.10)$$

and

$$a_{ij} = \frac{1}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right), \quad (4.1.1.11)$$

$$P = -\overline{u_i u_j} \frac{\partial U_i}{\partial x_j} = \frac{1}{2} P_{ii}, \quad (4.1.1.12)$$

$$G = -\beta g_i \overline{u_i \phi} = \frac{1}{2} G_{ii}. \quad (4.1.1.13)$$

The first contribution π_{ij}^1 to the pressure strain tensor is, therefore, proportional to the tensor a_{ij} , which we refer to as anisotropy tensor. It holds always that

$$a_{ii} = a_{11} + a_{22} + a_{33} = 0, \quad (4.1.1.14)$$

but in the case of isotropic turbulence, one has $u_\alpha u_\alpha = (2/3)k$ ($\alpha = 1, 2, 3$, summation not implied); therefore, $a_{\alpha\alpha} = 0$ ($\alpha = 1, 2, 3$). Thus, also, $\pi_{\alpha\alpha}^1 = 0$ in isotropic turbulence, and, in the general case, the components of the term π_{ij}^1 are a measure of the anisotropy of turbulence.

Similarly, the second contribution π_{ij}^2 is a measure of the anisotropy of the production of the stress $\overline{u_i u_j}$, due to the mean flow. In the case of isotropic turbulence, $P_{\alpha\alpha} = (2/3)p$ and therefore, $\pi_{aa}^2 = 0$. The third contribution is a measure of the anisotropy of production of the stress $\overline{u_i u_j}$, due to buoyancy forces. In the case of isotropic turbulence, $G_{\alpha\alpha} = 2G/3$; hence, $\pi_{\alpha\alpha}^3 = 0$. The fourth contribution π_{ij}^w takes into account the contributions of physical walls on the production of the stress $\overline{u_i u_j}$.

Assuming that local isotropy is at the high wave numbers at which dissipation occurs, we modeled the viscous dissipation tensor as follows:

$$\varepsilon_{ij} = 2\nu \frac{\partial \overline{u_i}}{\partial x_\ell} \frac{\partial \overline{u_j}}{\partial x_\ell} \approx \frac{2}{3} \varepsilon \delta_{ij}, \quad (4.1.1.15)$$

with

$$\varepsilon = \nu_\ell \frac{\partial \overline{u_n}}{\partial x_m} \frac{\partial \overline{u_n}}{\partial x_m}. \quad (4.1.1.16)$$

Inserting Eqs. 4.1.1.6, 4.1.1.8-4.1.1.10, and 4.1.1.15 into Eq. 4.1.1.1, we obtained the modeled transport equation for Reynolds stresses

$$\begin{aligned} \frac{\partial \overline{u_i u_j}}{\partial t} + U_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} = & \frac{\partial}{\partial x_\ell} \left(\nu_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} + c_s \frac{k^2}{\varepsilon} \frac{\partial \overline{u_i u_j}}{\partial x_\ell} \right) + P_{ij} + G_{ij} - c_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2k}{3} \delta_{ij} \right) \\ & - c_2 \frac{\varepsilon}{k} \left(P_{ij} - \frac{2}{3} P \delta_{ij} \right) - c_3 \frac{\varepsilon}{k} \left(G_{ij} - \frac{2}{3} G \delta_{ij} \right) + \pi_{ij}^w - \frac{2}{3} \varepsilon \delta_{ij}. \end{aligned} \quad (4.1.1.17)$$

Rearranging, we derive

$$\begin{aligned} \frac{\partial \overline{u_i u_j}}{\partial t} + U_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} = & \frac{\partial}{\partial x_\ell} \left(\nu_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} + c_s \frac{k^2}{\varepsilon} \frac{\partial \overline{u_i u_j}}{\partial x_\ell} \right) + P_{ij}(1 - c_2) + G_{ij}(1 - c_3) \\ & - c_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) + c_2 \frac{2}{3} P \delta_{ij} + c_3 \frac{2}{3} G \delta_{ij} + \pi_{ij}^w - \frac{2}{3} \varepsilon \delta_{ij}. \end{aligned} \quad (4.1.1.18)$$

Finally, using Eqs. 4.1.1.2, 4.1.1.3, 4.1.1.12, and 4.1.1.13, we obtain

$$\begin{aligned}
\frac{\partial \overline{u_i u_j}}{\partial t} + U_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} &= \frac{\partial}{\partial x_\ell} \left(v_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} + c_s \frac{k^2}{\varepsilon} \frac{\partial \overline{u_i u_j}}{\partial x_\ell} \right) - (1 - c_2) \left(\overline{u_i u_\ell} \frac{\partial U_j}{\partial x_\ell} + \overline{u_j u_\ell} \frac{\partial U_i}{\partial x_\ell} \right) \\
&\quad - (1 - c_3) (\beta g_i \overline{u_j \phi} + \beta g_j \overline{u_i \phi}) - c_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) \\
&\quad - c_2 \frac{2}{3} \overline{u_n u_m} \frac{\partial U_n}{\partial x_m} \delta_{ij} - c_3 \frac{2}{3} \beta g_\ell \overline{u_\ell \phi} \delta_{ij} + \pi_{ij}^w - \frac{2}{3} \varepsilon \delta_{ij}.
\end{aligned} \tag{4.1.1.19}$$

The numerical values of the constants are $c_s = 0.09$, $c_1 = 2.8$, $c_2 = 0.47$, and $c_3 = 0.47$.

It is easy to verify that summing the three equations (4.1.1.17) for $i = j$, we obtain the transport equation for $k = \overline{u_i u_i}/2$. Neglecting the terms that account for the wall effect, we have

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left(v_\ell \frac{\partial k}{\partial x_j} + c_s \frac{k^2}{\varepsilon} \frac{\partial k}{\partial x_j} \right) - \overline{u_i u_j} \frac{\partial U_i}{\partial x_j} - \beta g_j \overline{u_j \phi} - \varepsilon. \tag{4.1.1.20}$$

In this equation, the production terms (second and third on the right-hand side) are rigorous and not modeled. The turbulent diffusion coefficient is defined by

$$v_t = c_s \frac{k^2}{\varepsilon}. \tag{4.1.1.21}$$

4.1.2 Numerical Treatment

Equation 4.1.1.19 can be written in the compact form

$$\frac{\partial}{\partial t} \Phi_{ij} + \frac{\partial}{\partial x_\ell} J_\ell(\Phi_{ij}) = S_{ij}^R + S_{ij}^L, \tag{4.1.2.1}$$

with the following definitions:

$$\Phi_{ij} = \overline{u_i u_j}, \tag{4.1.2.2}$$

$$J_\ell(\Phi_{ij}) = U_\ell \Phi_{ij} - \Gamma_{\Phi_{ij}} \frac{\partial \Phi_{ij}}{\partial x_\ell} \quad (\text{corrective and diffusive flux}), \tag{4.1.2.3}$$

$$\Gamma_{\Phi_{ij}} = v_\ell + c_s \frac{k^2}{\varepsilon} \quad (\text{total diffusion coefficient}), \tag{4.1.2.4}$$

$$S_{ij}^R = -(1 - c_2) \left(\overline{u_i u_\ell} \frac{\partial U_j}{\partial x_\ell} + \overline{u_j u_\ell} \frac{\partial U_i}{\partial x_\ell} \right) - (1 - c_3) (\beta g_i \overline{u_j \phi} + \beta g_j \overline{u_i \phi}),$$

$$+ c_1 \frac{2}{3} \varepsilon \delta_{ij} - c_2 \frac{2}{3} \overline{u_n u_m} \frac{\partial U_n}{\partial x_m} \delta_{ij} - c_3 \frac{2}{3} \beta g_\ell \overline{u_\ell \phi} \delta_{ij} - \frac{2}{3} \varepsilon \delta_{ij}, \quad (4.1.2.5)$$

$$S_{ij}^L = c_1 \frac{\varepsilon}{k} \overline{u_i u_j}. \quad (4.1.2.6)$$

Superscripts R and L, used for the source terms, refer to the fact that, after discretization of Eq. 4.1.2.1, these terms are used, respectively, on the right- and left-hand sides of the equation.

To check and understand the code, we give the full expressions, with FORTRAN symbols, of the source term S_{ij}^R :

$$\begin{aligned} S_{ij}^R = & - (1 - c_2) \left(\underbrace{\overline{u_i u_1} \frac{\partial U_j}{\partial x_1} + \overline{u_i u_2} \frac{\partial U_j}{\partial x_2} + \overline{u_j u_3} \frac{\partial U_i}{\partial x_3}}_{\text{SUM11}} + \underbrace{\overline{u_j u_1} \frac{\partial U_i}{\partial x_1} + \overline{u_j u_2} \frac{\partial U_i}{\partial x_2} + \overline{u_i u_3} \frac{\partial U_j}{\partial x_3}}_{\text{SUM12}} \right) \\ & - \underbrace{(1 - c_3) (\beta g_1 \overline{u_j \phi} + \beta g_j \overline{u_i \phi})}_{\text{SCCU2}} - \underbrace{(1 - c_1) \frac{2}{3} \varepsilon \delta_{ij}}_{\text{SCCU3}} - \underbrace{c_3 \frac{2}{3} (\beta (g_1 \overline{u_1 \phi} + g_2 \overline{u_2 \phi} + g_3 \overline{u_3 \phi})) \delta_{ij}}_{\text{SCCU4}} \\ & - c_3 \frac{2}{3} \left[\underbrace{\overline{u_1 u_1} \frac{\partial U_1}{\partial x_1} + \overline{u_2 u_2} \frac{\partial U_2}{\partial x_2} + \overline{u_3 u_3} \frac{\partial U_3}{\partial x_3}}_{\text{SUM51}} + \underbrace{\overline{u_1 u_2} \left(\frac{\partial U_1}{\partial x_2} + \frac{\partial U_2}{\partial x_1} \right) + \overline{u_1 u_3} \left(\frac{\partial U_1}{\partial x_3} + \frac{\partial U_3}{\partial x_1} \right) + \overline{u_2 u_3} \left(\frac{\partial U_2}{\partial x_3} + \frac{\partial U_3}{\partial x_2} \right)}_{\text{SUM52}} \right] \\ = & - \underbrace{(1 - c_2) (\text{SUM11} + \text{SUM12})}_{\text{SCCU1}} - \underbrace{c_2 \frac{2}{3} (\text{SUM51} + \text{SUM52})}_{\text{SCCU5}} \\ = & - \text{SCCU1} - \text{SCCU2} - \text{SCCU3} - \text{SCCU4} - \text{SCCU5} \end{aligned} \quad (4.1.2.7)$$

the same way as Eq. 3.1.2.23. The volume integral of S_{ij}^L , which includes the dependent variable Φ_{ij} , is moved to the left-hand side of the discretized equation. The resulting linearEquation (4.1.2.7) is integrated over the volumes of the control cells and treated formally in ized algebraic equation for the Reynolds stresses is

$$a_o^{\Phi_{ij}} (\Phi_{ij})_o^{n+1} - \sum_1^6 \beta a_\beta^{\Phi_{ij}} (\Phi_{ij})_\beta^{n+1} = b_o^{\Phi_{ij}}, \quad (4.1.2.8)$$

where the coefficients are

$$a_o^{\Phi_{ij}} = \frac{V_o \rho_{fo}^{n+1}}{\Delta t} + c_1 \frac{2}{3} V_{fo} \rho_o^{n+1} [0, F_{i+1/2}] + [0, F_{j+1/2}] + [0, F_{k+1/2}]$$

$$\begin{aligned}
& + [0, -F_{i-1/2}] + [0, -F_{j-1/2}] + [0, -F_{k-1/2}] + D_{i+1/2}^{\Phi_{ij}} + D_{i-1/2}^{\Phi_{ij}} + D_{j+1/2}^{\Phi_{ij}} \\
& + D_{j-1/2}^{\Phi_{ij}} + D_{k+1/2}^{\Phi_{ij}} + D_{k-1/2}^{\Phi_{ij}}, \tag{4.1.2.9a}
\end{aligned}$$

$$a_1^{\Phi_{ij}} = [0, F_{i-1/2}] + D_{i-1/2}^{\Phi_{ij}}, \tag{4.1.2.9b}$$

$$a_2^{\Phi_{ij}} = [0, -F_{i+1/2}] + D_{i+1/2}^{\Phi_{ij}}, \tag{4.1.2.9c}$$

$$a_3^{\Phi_{ij}} = [0, F_{j-1/2}] + D_{j-1/2}^{\Phi_{ij}}, \tag{4.1.2.9d}$$

$$a_4^{\Phi_{ij}} = [0, -F_{j+1/2}] + D_{j+1/2}^{\Phi_{ij}}, \tag{4.1.2.9e}$$

$$a_5^{\Phi_{ij}} = [0, F_{k-1/2}] + D_{k-1/2}^{\Phi_{ij}}, \tag{4.1.2.9f}$$

$$a_6^{\Phi_{ij}} = [0, -F_{k+1/2}] + D_{k+1/2}^{\Phi_{ij}}, \tag{4.1.2.9g}$$

$$b_o^{\Phi_{ij}} = V_{f_o} \frac{(\rho \Phi_{ij})_o^n}{\Delta t} + V_{f_o} \rho_o^{n+1} \langle S_{ij}^R \rangle_3^{n+1}. \tag{4.1.2.9h}$$

The diffusion coefficients are given by equations that are formally identical to Eq. 3.1.36.

Again, using the discretized form of the continuity equation Eq. 3.1.41, we obtain the so-called second form of the coefficient a_o , i.e.,

$$\begin{aligned}
a_o^{\Pi \Phi_{ij}} = & \frac{V_{f_o} \rho_o^n}{\Delta t} + c_1 \frac{\epsilon}{k} V_{f_o} \rho_o^{n+1} + [0, F_{i-1/2}] + [0, -F_{i+1/2}] + [0, F_{j-1/2}] + [0, -F_{j+1/2}] \\
& + [0, F_{k-1/2}] + [0, -F_{k+1/2}] \\
& + D_{i+1/2}^{\Phi_{ij}} + D_{j+1/2}^{\Phi_{ij}} + D_{k+1/2}^{\Phi_{ij}} + D_{i-1/2}^{\Phi_{ij}} + D_{j-1/2}^{\Phi_{ij}} + D_{k-1/2}^{\Phi_{ij}}. \tag{4.1.2.10}
\end{aligned}$$

4.1.3 Boundary Conditions

We use the boundary conditions for both the laminar sublayer ($y_p < y_\ell$) and the turbulent layer ($y_p \geq y_\ell$).

$$\overline{(u_i u_j)}_p = \frac{2}{3} \frac{u_*^2}{\sqrt{c_\mu}} \quad (i = j) \tag{4.1.3.1}$$

and

$$(\overline{u_i u_j})_p = -u^{*2}, \quad (i \neq j), \quad (4.1.3.2)$$

where the u^* is friction velocity.

Equations 4.1.3.1 and 4.1.3.2 are consistent with the boundary condition

$$k_p = \frac{u^{*2}}{\sqrt{c_\mu}}, \quad (4.1.3.3)$$

which is used in the k - ε model, as is evident from the definition of turbulent kinetic energy $k_p = \frac{1}{2}(\overline{u_i u_i})$.

4.2 Transport Equation for Dissipation of Turbulent Kinetic Energy

4.2.1 Analytical Treatment

The transport equation that describes the space and time distribution of the dissipation of turbulent kinetic energy ε is

$$\rho \frac{\partial(\rho\varepsilon)}{\partial t} + \rho U_j \frac{\partial\varepsilon}{\partial x_j} = c_{1\varepsilon} \frac{\varepsilon}{k} (P_k + G_k)(1 + c_{3\varepsilon} R_f) - c_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_j} \left(\mu_\ell \frac{\partial\varepsilon}{\partial x_j} + c_\varepsilon \rho \frac{k}{\varepsilon} \overline{u_j u_m} \frac{\partial\varepsilon}{\partial x_m} \right). \quad (4.2.1.1)$$

In this equation,

$$R_f = - \frac{G_k}{P_k} \quad (4.2.1.2)$$

is the Richardson number. The numerical value of the constants is $c_{1\varepsilon} = 1.44$, $c_{2\varepsilon} = 1.92$, $c_{3\varepsilon} = 0.8$ and $c_\varepsilon = 0.15$.

Using the continuity equation and the definition of the source term

$$S_\varepsilon = c_{1\varepsilon} \frac{\varepsilon}{k} (P_k + G_k) (1 + c_{3\varepsilon} R_f) - c_{2\varepsilon} \rho \frac{\varepsilon^2}{k}, \quad (4.2.1.3)$$

we can rewrite Eq. 4.2.1.1 as

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial}{\partial x_j} \left(\rho U_j \varepsilon - \mu_\ell \frac{\partial\varepsilon}{\partial x_j} - c_\varepsilon \rho \frac{k}{\varepsilon} \overline{u_j u_m} \frac{\partial\varepsilon}{\partial x_m} \right) = S_\varepsilon. \quad (4.2.1.4)$$

Let us define the convective, diffusive (laminar and turbulent), and total (convective plus diffusive) fluxes as follows:

$$J_{ej}^c = \rho U_j \epsilon, \quad (4.2.1.5)$$

$$J_{ej}^{d\ell} = -\mu_\ell \frac{\partial \epsilon}{\partial x_j}, \quad (4.2.1.6)$$

$$J_{ej}^{dt} = c_\epsilon \rho \frac{k}{\epsilon} \overline{u_j u_m} \frac{\partial \epsilon}{\partial x_m} = -\Gamma_{ejm} \frac{\partial \epsilon}{\partial x_m}, \quad (4.2.1.7)$$

$$J_{ej} = \rho U_j \epsilon - \mu_\ell \frac{\partial \epsilon}{\partial x_j} - \Gamma_{ejm} \frac{\partial \epsilon}{\partial x_m} = J_{ej}^c + J_{ej}^{d\ell} + J_{ej}^{dt}, \quad (4.2.1.8)$$

with

$$\Gamma_{ejm} = c_\epsilon \rho \frac{k}{\epsilon} \overline{u_j u_m}. \quad (4.2.1.9)$$

With these definitions, Eq. 4.2.1.4 can be written in the compact form

$$\frac{\partial(\rho\epsilon)}{\partial t} + \frac{\partial}{\partial x_j} J_{ej} = S_\epsilon. \quad (4.2.1.10)$$

Integration of Eq. 4.2.1.10 over the volume V_f and application of the Gauss theorem yields

$$\begin{aligned} \int_{V_f} \frac{\partial(\rho\epsilon)}{\partial t} dV + \int_{A_{f,i+1/2}} J_{ei} dA - \int_{A_{f,i-1/2}} J_{ei} dA + \int_{A_{f,j+1/2}} J_{ej} dA - \int_{A_{f,j-1/2}} J_{ej} dA \\ + \int_{A_{f,k+1/2}} J_{ek} dA - \int_{A_{f,k-1/2}} J_{ek} dA = \int_{V_f} S_\epsilon dV. \end{aligned} \quad (4.2.1.11)$$

4.2.2 Numerical Treatment

Equation 4.2.1.11 is discretized as follows:

$$\begin{aligned} \frac{V_{f0}}{\Delta t} \left[(\rho\epsilon)_o^{n+1} - (\rho\epsilon)_o^n \right] + \left\langle J_\epsilon^c A_f \right\rangle_{\alpha+1/2}^{n+1} - \left\langle J_\epsilon^c A_f \right\rangle_{\alpha-1/2}^{n+1} + \left\langle (J_\epsilon^{d\ell} + J_\epsilon^{dt}) A_f \right\rangle_{\alpha+1/2}^{n+1} \\ - \left\langle (J_\epsilon^{d\ell} + J_\epsilon^{dt}) A_f \right\rangle_{\alpha-1/2}^{n+1} = V_f \langle S_\epsilon^{n+1} \rangle_3, \end{aligned} \quad (4.2.2.1)$$

where summation for $\alpha = i, j, k$ is implied.

The convective terms are computed as follows:

$$\langle J_{\varepsilon}^c A_f \rangle_{\alpha+1/2}^{n+1} = \langle \rho U \varepsilon A_f \rangle_{\alpha+1/2}^{n+1} = \langle F \varepsilon \rangle_{\alpha+1/2}^{n+1} = [0, F_{\alpha+1/2}] \varepsilon_{\alpha}^{n+1} - [0, -F_{\alpha+1/2}] \varepsilon_{\alpha+1}^{n+1}, \quad (4.2.2.2a)$$

$$\langle J_{\varepsilon}^c A_f \rangle_{\alpha-1/2}^{n+1} = [0, F_{\alpha-1/2}] \varepsilon_{\alpha-1}^{n+1} - [0, -F_{\alpha-1/2}] \varepsilon_{\alpha}^{n+1}. \quad (4.2.2.2b)$$

The diffusive terms are computed, letting $Z = c_{\varepsilon} \rho k / \varepsilon$, by

$$\begin{aligned} \langle (J_{\varepsilon}^{d\ell} + J_{\varepsilon}^{dt}) A_f \rangle_{i+1/2} &= \left\langle \left(-\mu_{\ell} \frac{\partial \varepsilon}{\partial x_j} - \Gamma_{\varepsilon j m} \frac{\partial \varepsilon}{\partial x_m} \right) A_f \right\rangle_{i+1/2} \\ &= -A_{f,i+1/2} \left[\left(\overline{Z u_1 u_1} + \mu_{\ell} \right) \frac{\partial \varepsilon}{\partial x_1} + \overline{Z u_1 u_2} \frac{\partial \varepsilon}{\partial x_2} + \overline{Z u_1 u_3} \frac{\partial \varepsilon}{\partial x_3} \right]_{i+1/2} \end{aligned} \quad (4.2.2.3a)$$

$$\begin{aligned} \langle (J_{\varepsilon}^{d\ell} + J_{\varepsilon}^{dt}) A_f \rangle_{j+1/2} &= -A_{f,j+1/2} \left[\overline{Z u_2 u_1} \frac{\partial \varepsilon}{\partial x_1} + \left(\overline{Z u_2 u_2} + \mu_{\ell} \right) \frac{\partial \varepsilon}{\partial x_2} + \overline{Z u_2 u_3} \frac{\partial \varepsilon}{\partial x_3} \right]_{j+1/2} \\ &\quad (4.2.2.3b) \end{aligned}$$

$$\begin{aligned} \langle (J_{\varepsilon}^{d\ell} + J_{\varepsilon}^{dt}) A_f \rangle_{k+1/2} &= -A_{f,k+1/2} \left[\overline{Z u_3 u_1} \frac{\partial \varepsilon}{\partial x_1} + \overline{Z u_3 u_2} \frac{\partial \varepsilon}{\partial x_2} + \left(\overline{Z u_3 u_3} + \mu_{\ell} \right) \frac{\partial \varepsilon}{\partial x_3} \right]_{k+1/2} \\ &\quad (4.2.2.3c) \end{aligned}$$

and similarly for $i-1/2$, $j-1/2$, and $k-1/2$.

Inserting Eqs. 4.2.2.2 and 4.2.2.3 into Eq. 4.2.2.1, we obtain (replacing x, y, z for x_1, x_2, x_3)

$$\begin{aligned} &\frac{V_f}{\Delta t} \left[(\rho \varepsilon)^{n+1} - (\rho \varepsilon)^n \right]_{ijk} \\ &+ [0, F_{i+1/2}] \varepsilon_{ijk}^{n+1} - [0, -F_{i+1/2, jk}] \varepsilon_{i+1}^{n+1} - [0, F_{i-1/2}] \varepsilon_{i-1}^{n+1} + [0, -F_{i-1/2}] \varepsilon_{ijk}^{n+1} \\ &+ [0, F_{j+1/2}] \varepsilon_{ijk}^{n+1} - [0, -F_{j+1/2}] \varepsilon_{j+1}^{n+1} - [0, F_{j-1/2}] \varepsilon_{j-1}^{n+1} + [0, -F_{j-1/2}] \varepsilon_{ijk}^{n+1} \\ &+ [0, F_{k+1/2}] \varepsilon_{ijk}^{n+1} - [0, -F_{k+1/2}] \varepsilon_{k+1}^{n+1} - [0, F_{k-1/2}] \varepsilon_{k-1}^{n+1} + [0, -F_{k-1/2}] \varepsilon_{ijk}^{n+1} \\ &= V_{fo} < S_{\varepsilon} >_{ijk}^{n+1} \end{aligned}$$

$$\begin{aligned}
& + \frac{A_{f,i+1/2}}{\Delta x_{i+1/2}} (\overline{Zu_1u_1} + \mu_\ell)_{i+1/2} (\varepsilon_{i+1}^{n+1} - \varepsilon_i^{n+1}) + A_{f,i+1/2} \left(\overline{Zu_1u_1} \frac{\partial \varepsilon}{\partial y} + \overline{Zu_1u_3} \frac{\partial \varepsilon}{\partial z} \right)_{i+1/2} \\
& - \frac{A_{f,i-1/2}}{\Delta x_{i-1/2}} (\overline{Zu_1u_1} + \mu_\ell)_{i-1/2} (\varepsilon_i^{n+1} - \varepsilon_{i-1}^{n+1}) - A_{f,i-1/2} \left(\overline{Zu_1u_2} \frac{\partial \varepsilon}{\partial y} + \overline{Zu_1u_3} \frac{\partial \varepsilon}{\partial z} \right)_{i-1/2} \\
& + \frac{A_{f,j+1/2}}{\Delta y_{j+1/2}} (\overline{Zu_2u_2} + \mu_\ell)_{j+1/2} (\varepsilon_{j+1}^{n+1} - \varepsilon_j^{n+1}) + A_{f,j+1/2} \left(\overline{Zu_2u_1} \frac{\partial \varepsilon}{\partial x} + \overline{Zu_2u_3} \frac{\partial \varepsilon}{\partial z} \right)_{j+1/2} \\
& - \frac{A_{f,j-1/2}}{\Delta y_{j-1/2}} (\overline{Zu_2u_2} + \mu_\ell)_{j-1/2} (\varepsilon_j^{n+1} - \varepsilon_{j-1}^{n+1}) - A_{f,j-1/2} \left(\overline{Zu_2u_1} \frac{\partial \varepsilon}{\partial x} + \overline{Zu_2u_3} \frac{\partial \varepsilon}{\partial z} \right)_{j-1/2} \\
& + \frac{A_{f,k+1/2}}{\Delta z_{k+1/2}} (\overline{Zu_3u_3} + \mu_\ell)_{k+1/2} (\varepsilon_{k+1}^{n+1} - \varepsilon_k^{n+1}) + A_{f,k+1/2} \left(\overline{Zu_3u_1} \frac{\partial \varepsilon}{\partial x} + \overline{Zu_3u_2} \frac{\partial \varepsilon}{\partial y} \right)_{k+1/2} \\
& - \frac{A_{f,k-1/2}}{\Delta z_{k-1/2}} (\overline{Zu_3u_3} + \mu_\ell)_{k-1/2} (\varepsilon_k^{n+1} - \varepsilon_{k-1}^{n+1}) - A_{f,k-1/2} \left(\overline{Zu_3u_1} \frac{\partial \varepsilon}{\partial x} + \overline{Zu_3u_2} \frac{\partial \varepsilon}{\partial y} \right)_{k-1/2}.
\end{aligned} \tag{4.2.2.4}$$

Using the definitions of the diffusion coefficients

$$D_{i+1/2}^\varepsilon = \frac{A_{f,i+1/2}}{\Delta x_{i+1/2}} (\overline{Zu_1u_1} + \mu_\ell), \tag{4.2.2.5a}$$

$$D_{j+1/2}^\varepsilon = \frac{A_{f,j+1/2}}{\Delta y_{j+1/2}} (\overline{Zu_2u_2} + \mu_\ell), \tag{4.2.2.5b}$$

$$D_{k+1/2}^\varepsilon = \frac{A_{f,k+1/2}}{\Delta z_{k+1/2}} (\overline{Zu_3u_3} + \mu_\ell), \tag{4.2.2.5c}$$

and similar ones for $i-1/2$, $j-1/2$, $k-1/2$, and rearranging, we obtain

$$\begin{aligned}
& \varepsilon_0^{n+1} \left\{ \frac{V_f \rho_0^{n+1}}{\Delta t} + [0, F_{i+1/2}] + [0, F_{j+1/2}] + [0, F_{k+1/2}] \right. \\
& + [0, -F_{i-1/2}] + [0, -F_{j-1/2}] + [0, -F_{k-1/2}] \\
& \left. + D_{i+1/2}^\varepsilon + D_{j+1/2}^\varepsilon + D_{k+1/2}^\varepsilon + D_{i-1/2}^\varepsilon + D_{j-1/2}^\varepsilon + D_{k-1/2}^\varepsilon \right\} \\
& - \varepsilon_1^{n+1} \left\{ [0, F_{i-1/2}] + D_{i-1/2}^\varepsilon \right\} - \varepsilon_2^{n+1} \left\{ [0, -F_{i+1/2}] + D_{i+1/2}^\varepsilon \right\}
\end{aligned}$$

$$\begin{aligned}
& -\varepsilon_3^{n+1} \left\{ [0, F_{j-1/2}] + D_{j-1/2}^\varepsilon \right\} - \varepsilon_4^{n+1} \left\{ [0, -F_{j+1/2}] + D_{j+1/2}^\varepsilon \right\} \\
& - \varepsilon_5^{n+1} \left\{ [0, F_{k-1/2}] + D_{k-1/2}^\varepsilon \right\} - \varepsilon_6^{n+1} \left\{ [0, -F_{k+1/2}] + D_{k+1/2}^\varepsilon \right\} \\
& = \frac{V_{f0}}{\Delta t} (\rho\varepsilon)_0^n + V_{f0} < S_\varepsilon >_3^{n+1} \\
& + A_{f,i+1/2} \left(\overline{Zu_1u_1} \frac{\partial\varepsilon}{\partial y} + \overline{Zu_1u_3} \frac{\partial\varepsilon}{\partial z} \right)_{i+1/2} - A_{f,i-1/2} \left(\overline{Zu_1u_2} \frac{\partial\varepsilon}{\partial y} + \overline{Zu_1u_3} \frac{\partial\varepsilon}{\partial z} \right)_{i-1/2} \\
& + A_{f,i+1/2} \left(\overline{Zu_2u_1} \frac{\partial\varepsilon}{\partial x} + \overline{Zu_2u_3} \frac{\partial\varepsilon}{\partial z} \right)_{i+1/2} - A_{f,i-1/2} \left(\overline{Zu_2u_1} \frac{\partial\varepsilon}{\partial x} + \overline{Zu_2u_3} \frac{\partial\varepsilon}{\partial z} \right)_{i-1/2} \\
& + A_{f,k+1/2} \left(\overline{Zu_3u_1} \frac{\partial\varepsilon}{\partial x} + \overline{Zu_3u_2} \frac{\partial\varepsilon}{\partial y} \right)_{k+1/2} - A_{f,k-1/2} \left(\overline{Zu_3u_1} \frac{\partial\varepsilon}{\partial x} + \overline{Zu_3u_2} \frac{\partial\varepsilon}{\partial y} \right)_{k-1/2}.
\end{aligned} \tag{4.2.2.6}$$

Eq. 4.2.2.6 can be written in the compact form

$$a_o^\varepsilon \varepsilon_o^{n+1} - \sum_1^6 a_\beta^\varepsilon \varepsilon_\beta^{n+1} = b_o^\varepsilon, \tag{4.2.2.7}$$

with the following definition of the coefficients:

$$\begin{aligned}
a_o^\varepsilon &= \frac{V_{f0}}{\Delta t} \rho_o^{n+1} + [0, F_{i+1/2}] + [0, F_{j+1/2}] + [0, F_{k+1/2}] + [0, -F_{i-1/2}] + [0, -F_{j-1/2}] \\
&+ [0, -F_{k-1/2}] + D_{i+1/2}^\varepsilon + D_{j+1/2}^\varepsilon + D_{k+1/2}^\varepsilon + D_{i-1/2}^\varepsilon + D_{j-1/2}^\varepsilon + D_{k-1/2}^\varepsilon,
\end{aligned} \tag{4.2.2.8a}$$

$$a_1^\varepsilon = [0, F_{i-1/2}], \tag{4.2.2.8b}$$

$$a_2^\varepsilon = [0, -F_{i+1/2}], \tag{4.2.2.8c}$$

$$a_3^\varepsilon = [0, F_{j-1/2}], \tag{4.2.2.8d}$$

$$a_4^\varepsilon = [0, -F_{j+1/2}], \tag{4.2.2.8e}$$

$$a_5^\varepsilon = [0, F_{k-1/2}], \tag{4.2.2.8f}$$

$$a_6^\varepsilon = [0, -F_{k+1/2}], \tag{4.2.2.8g}$$

$$b_o^\varepsilon = \frac{V_{f0}}{\Delta t} (\rho\varepsilon)_0^n + V_{f0} < S_\varepsilon >_3^{n+1}$$

$$\begin{aligned}
& + A_{f,i+1/2} \left(\overline{Zu_1u_1} \frac{\partial \varepsilon}{\partial y} + \overline{Zu_1u_3} \frac{\partial \varepsilon}{\partial z} \right)_{i+1/2} - A_{f,i-1/2} \left(\overline{Zu_1u_2} \frac{\partial \varepsilon}{\partial y} + \overline{Zu_1u_3} \frac{\partial \varepsilon}{\partial z} \right)_{i-1/2} \\
& + A_{f,i+1/2} \left(\overline{Zu_2u_1} \frac{\partial \varepsilon}{\partial x} + \overline{Zu_2u_3} \frac{\partial \varepsilon}{\partial z} \right)_{i+1/2} - A_{f,i-1/2} \left(\overline{Zu_2u_1} \frac{\partial \varepsilon}{\partial x} + \overline{Zu_2u_3} \frac{\partial \varepsilon}{\partial z} \right)_{i-1/2} \\
& + A_{f,k+1/2} \left(\overline{Zu_3u_1} \frac{\partial \varepsilon}{\partial x} + \overline{Zu_3u_2} \frac{\partial \varepsilon}{\partial y} \right)_{k+1/2} - A_{f,k-1/2} \left(\overline{Zu_3u_1} \frac{\partial \varepsilon}{\partial x} + \overline{Zu_3u_2} \frac{\partial \varepsilon}{\partial y} \right)_{k-1/2} .
\end{aligned} \tag{4.2.2.8h}$$

Using the discretized continuity equation Eq. 3.1.4.1 we obtain the second form of the coefficient as

$$\begin{aligned}
a_o^{IIe} = & \frac{V_{fo}}{\Delta t} \rho_o^n + [0, F_{i-1/2}] + [0, -F_{i+1/2}] + [0, F_{j-1/2}] + [0, -F_{j+1/2}] + [0, F_{k-1/2}] \\
& + [0, -F_{k+1/2}] + D_{i+1/2} + D_{j+1/2} + D_{k+1/2} + D_{i-1/2} + D_{j-1/2} + D_{k-1/2} .
\end{aligned} \tag{4.2.2.9}$$

4.2.3 Boundary Conditions

With reference to Figs. 1 and 2, when $y_p > y_\ell$, the first node is in the fully turbulent zone and it holds that

$$\varepsilon_p = u^{*3} / (Ky_p) \tag{4.2.3.1}$$

and

$$u^* = KU_p / \ln(Ey_p u^* / \nu_\ell) . \tag{4.2.3.2}$$

When $y_p \leq y_\ell$ the node P is in the laminar sublayer, and one has

$$\varepsilon_p = u^{*3} / (Ky_\ell) , \tag{4.2.3.3}$$

where K ($= 0.42$) is the von Karman constant and E ($= 9.0$) is a constant that is dependent on the roughness of the wall.

4.3 Momentum Equations

4.3.1 Analytical Treatment

The momentum equations used in combination with the RSM are

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j U_i) = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu_\ell \frac{\partial U_i}{\partial x_j} - \rho \overline{u_i u_j} \right) + \rho g_i = R_i . \tag{4.3.1.1}$$

Let us define the convective, diffusive (laminar and turbulent), and total (convective plus diffusive) momentum fluxes by

$$J_{mij}^c = \rho U_j U_i, \quad (4.3.1.2)$$

$$J_{mij}^{d\ell} = -\mu_\ell \frac{\partial U_i}{\partial x_j}, \quad (4.3.1.3)$$

$$J_{mij}^{dt} = \rho \overline{u_i u_j}, \quad (4.3.1.4)$$

$$J_{mij} = \rho U_j U_i - \mu_\ell \frac{\partial U_i}{\partial x_j} + \rho \overline{u_i u_j} = J_{mij}^c + J_{mij}^{d\ell} + J_{mij}^{dt}. \quad (4.3.1.5)$$

If we define a source term by

$$S_{mi} = \rho g_i - \frac{\partial p}{\partial x_i} - R_i, \quad (4.3.1.6)$$

Eq. 4.3.1.1 can be written in the compact form

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial J_{mij}}{\partial x_j} = S_{mi}. \quad (4.3.1.7)$$

Integration of Eq. 4.3.1.7 over the volume $V_{f,i+1/2}$ of a staggered mesh (displaced by one-half of a mesh in the i direction) and application of the Green theorem yields

$$\int_{V_{f,i-1/2}} \frac{\partial(\rho U_i)}{\partial t} dV + \int_{A_{f,\alpha+1/2}} J_{mi\alpha} dA - \int_{A_{f,\alpha-1/2}} J_{mi\alpha} dA = \int_{V_{f,\alpha-1/2}} S_{mi} dV. \quad (4.3.1.8)$$

Summation is implied over $\alpha = (i, j, k)$.

4.3.2 Numerical Treatment

Let us use the subscript "o" for the displaced mesh over which volume integration has been performed. Eq. 4.3.1.8 is discretized as follows:

$$\begin{aligned} & V_{fo} \left[\rho_o^n \frac{(U_{io}^{n+1} - U_{io}^n)}{\Delta t} + U_{io}^n \left(\frac{\partial \rho}{\partial t} \right)_o^n \right] + \langle J_{mi\alpha}^c A_f \rangle_{\alpha+1/2}^{n+1} - \langle J_{mi\alpha}^c A_f \rangle_{\alpha-1/2}^{n+1} \\ & + \langle J_{mi\alpha}^{d\ell} A_f \rangle_{\alpha+1/2}^{n+1} - \langle J_{mi\alpha}^{d\ell} A_f \rangle_{\alpha-1/2}^{n+1} + \langle J_{mi\alpha}^{dt} A_f \rangle_{\alpha+1/2}^{n+1} - \langle J_{mi\alpha}^{dt} A_f \rangle_{\alpha-1/2}^{n+1} \\ & = V_{fo} \langle S_{mi} \rangle_3. \end{aligned} \quad (4.3.2.1)$$

The convective fluxes are computed by

$$\begin{aligned}
\langle J_{\text{mix}}^c A_f \rangle_{\alpha+1/2}^{n+1} &= \langle \rho U_\alpha U_i A_f \rangle_{\alpha+1/2}^{n+1} = \langle F U_{i\alpha} \rangle_{\alpha+1/2}^{n+1} \\
&= [0, F_{\alpha+1/2}] U_{i\alpha}^{n+1} - [0, -F_{\alpha-1/2}] U_{i,\alpha+1}^{n+1},
\end{aligned} \tag{4.3.2.2a}$$

$$\langle J_{\text{mix}}^c A_f \rangle_{\alpha-1/2}^{n+1} = [0, F_{\alpha-1/2}] U_{i,\alpha-1}^{n+1} - [0, -F_{\alpha-1/2}] U_{i\alpha}^{n+1}. \tag{4.3.2.2b}$$

The diffusive laminar fluxes are computed by

$$\begin{aligned}
\langle J_{\text{mix}}^{d\ell} A_f \rangle_{\alpha+1/2}^{n+1} &= - \left\langle \mu_\ell \frac{\partial U_i}{\partial x_\alpha} A_f \right\rangle_{\alpha+1/2}^{n+1} = - \frac{A_{f,\alpha+1/2} (U_{i,\alpha+1} - U_{i\alpha})^{n+1}}{\frac{1}{2} \left(\frac{\Delta x_\alpha}{\mu_{\ell\alpha}} + \frac{\Delta x_{\alpha+1}}{\mu_{\ell,\alpha+1}} \right)} \\
&= - D_{\alpha+1/2}^{m\ell} (U_{i,\alpha+1} - U_{i\alpha})^{n+1},
\end{aligned} \tag{4.3.2.3a}$$

$$\begin{aligned}
\langle J_{\text{mix}}^{d\ell} A_f \rangle_{\alpha-1/2}^{n+1} &= - \left\langle \mu_\ell \frac{\partial U_i}{\partial x_\alpha} A_f \right\rangle_{\alpha-1/2}^{n+1} \\
&= - \frac{A_{f,\alpha-1/2} (U_{i\alpha} - U_{i,\alpha-1})^{n+1}}{\frac{1}{2} \left(\frac{\Delta x_{\alpha-1}}{\mu_{\ell,\alpha-1}} + \frac{\Delta x_\alpha}{\mu_{\ell,\alpha}} \right)} = - D_{\alpha-1/2}^{m\ell} (U_{i\alpha} - U_{i,\alpha-1})^{n+1}.
\end{aligned} \tag{4.3.2.3b}$$

The definition of the diffusive coefficients $D^{m\ell}$ is formally identical with that of Eq. 3.1.36, but replacing Γ with μ_ℓ .

The diffusive turbulent fluxes are computed by:

$$\langle J_{\text{mix}}^{dt} A_f \rangle_{\alpha-1/2}^{n+1} = \langle \overline{\rho u_i u_\alpha} A_f \rangle_{\alpha-1/2}^{n+1}. \tag{4.3.2.4}$$

The computation of these terms is explained in detail in the next section.

The volume integral of the source term, given by Eq. 4.3.1.6, can be computed as follows:

$$\int_{V_{fo}} S_{\text{mi}} dV = V_{fo} \langle S_{\text{mi}} \rangle_3 = V_{fo} \langle \rho g_i \rangle_3 - V_{fo} \frac{\langle R_i \rangle_3}{U_{io}^n} U_{io}^{n+1} - d_o^i (p_{i+1}^{n+1} - p_o^{n+1}), \tag{4.3.2.5}$$

where

$$d_o^i = (\gamma_o + \gamma_{i+1}) \Delta \ell_j \Delta \ell_k / 2. \tag{4.3.2.6}$$

The second term on the right-hand side of Eq. 4.3.1.5 implies a linearization of the drag forces, which depend on U_i . The third term arises from the volume integration of the pressure gradient $\partial p / \partial x_i$. γ in Eq. 4.3.1.6 is the surface permeability.

Inserting Eqs. 4.3.2.2-4.3.2.5 into Eq. 4.3.2.1, we obtain

$$\begin{aligned}
 V_{fo} \left[\rho_o^n \frac{(U_{io}^{n+1} - U_{io}^n)}{\Delta t} + U_{io}^n \left(\frac{\partial \rho}{\partial t} \right)_o^n \right] &+ [0, F_{\alpha+1/2}] U_{io}^{n+1} - [0, -F_{\alpha+1/2}] U_{i,\alpha+1}^{n+1} \\
 &- [0, F_{\alpha-1/2}] U_{i,\alpha-1}^{n+1} + [0, -F_{\alpha-1/2}] U_{io}^{n+1} - D_{\alpha+1/2}^{m\ell} (U_{i,\alpha+1} - U_{io})^{n+1} \\
 &+ D_{\alpha-1/2}^{m\ell} (U_{io}^{n+1} - U_{i,\alpha-1}^{n+1}) + \langle \rho u_i u_\alpha A_f \rangle_{\alpha+1/2}^{n+1} - \langle \rho u_i u_\alpha A_f \rangle_{\alpha-1/2}^{n+1} \\
 &= V_{fo} \langle \rho g_i \rangle_3 - V_{fo} \frac{\langle R_i \rangle_3}{U_{io}^n} U_{io}^{n+1} - d_o^i (p_{i+1}^{n+1} - p_o^{n+1}). \quad (4.3.2.7)
 \end{aligned}$$

Rearranging Eq. 4.3.2.7, we obtain

$$\begin{aligned}
 U_{io}^{n+1} \left\{ V_{fo} \frac{\rho_o^n}{\Delta t} + V_{fo} \frac{\langle R_i \rangle_3}{U_{io}^n} + [0, F_{\alpha+1/2}] + [0, -F_{\alpha-1/2}] + D_{\alpha+1/2}^{m\ell} + D_{\alpha-1/2}^{m\ell} \right\} \\
 - U_{i,\alpha+1}^{n+1} \{ [0, -F_{\alpha+1/2}] + D_{\alpha+1/2}^{m\ell} \} - U_{i,\alpha-1}^{n+1} \{ [0, F_{\alpha-1/2}] + D_{\alpha-1/2}^{m\ell} \} + d_o^i (p_{i+1}^{n+1} - p_o^{n+1}) \\
 = V_{fo} \rho_o^n \frac{U_{io}^n}{\Delta t} - V_{fo} U_{io}^n \left(\frac{\partial \rho}{\partial t} \right)_o^n + V_{fo} \langle \rho g_i \rangle_3 - \langle \rho u_i u_\alpha A_f \rangle_{\alpha+1/2}^{n+1} + \langle \rho u_i u_\alpha A_f \rangle_{\alpha-1/2}^{n+1}. \quad (4.3.2.8)
 \end{aligned}$$

4.3.3 Computation of Turbulent Fluxes, Explicit Formulation

The turbulent fluxes, i.e., the last two terms of Eq. 4.3.2.8, are computed with the last available iterative values of the Reynolds stresses $\overline{u_i u_j}$. Because these terms do not contain the unknown U_{io} , they are brought to the right-hand side of Eq. 4.3.2.8 and considered as a contribution to the source term. For this reason, the computation of these terms is referred to as explicit. The possibility of an implicit formulation is explained in the next section. Because the computation of the turbulent fluxes is the model feature of the RSM, we present all of the details and FORTRAN symbols that are used for the coding.

In the following, both of the sets of subscripts (1,2,3) and (i,j,k) refer to the (x,y,z) coordinate directions. Let us consider first the x component of the momentum equation, for a control volume indexed as (i+1/2, j, k). The full expression of the turbulent fluxes on the right-hand side of Eq. 4.3.2.8 is (overbars are replaced by the symbol < >):

$$\begin{aligned}
 RSTU = &- A_{f,i+1/2,j+1/2,k} \langle \rho \overline{u_1 u_2} \rangle_{i+1/2,j+1/2,k} + A_{f,i+1/2,j-1/2,k} \langle \rho \overline{u_1 u_2} \rangle_{i+1/2,j-1/2,k} \\
 &- A_{f,i+1/2,j,k+1/2} \langle \rho \overline{u_1 u_3} \rangle_{i+1/2,j,k+1/2} + A_{f,i+1/2,j,k-1/2} \langle \rho \overline{u_1 u_3} \rangle_{i+1/2,j,k-1/2} \\
 &- A_{f,i+1,j,k} \langle \rho \overline{u_1 u_1} \rangle_{i+1,j,k} + A_{f,ijk} \langle \rho \overline{u_1 u_1} \rangle_{ijk}. \quad (4.3.3.1)
 \end{aligned}$$

Similarly, for the y direction and for a control volume indexed $(i, j+1/2, k)$ we have

$$\begin{aligned} \text{RSTV} = & -A_{f,i+1/2,j+1/2,k} \langle \overline{\rho u_2 u_1} \rangle_{i+1/2,j+1/2,k} + [A_f \langle \overline{\rho u_2 u_1} \rangle]_{i-1/2,j+1/2,k} \\ & - [A_f \langle \overline{\rho u_2 u_2} \rangle]_{i,j+1,k} + [A_f \langle \overline{\rho u_2 u_2} \rangle]_{ijk} \\ & - [A_f \langle \overline{\rho u_2 u_3} \rangle]_{i,j+1/2,k+1/2} + [A_f \langle \overline{\rho u_2 u_3} \rangle]_{i,j+1/2,k-1/2}. \end{aligned} \quad (4.3.3.2)$$

For the z direction and a control volume indexed $(i, j, k+1/2)$ we have

$$\begin{aligned} \text{RSTW} = & -A_{f,i+1/2,j,k+1/2} \langle \overline{\rho u_3 u_1} \rangle_{i+1/2,j,k+1/2} + A_{f,i-1/2,j,k+1/2} \langle \overline{\rho u_3 u_1} \rangle_{i-1/2,j,k+1/2} \\ & - A_{f,i,j+1/2,k+1/2} \langle \overline{\rho u_3 u_2} \rangle_{i,j+1/2,k+1/2} + A_{f,i,j-1/2,k+1/2} \langle \overline{\rho u_3 u_2} \rangle_{i,j-1/2,k+1/2} \\ & - A_{f,i,j,k+1} \langle \overline{\rho u_3 u_3} \rangle_{i,j,k+1} + A_{f,i,j,k} \langle \overline{\rho u_3 u_3} \rangle_{ijk}. \end{aligned} \quad (4.3.3.3)$$

The terms in RSTU are computed as follows:

We allow a shorter notation

$$f^{ij} = \overline{\rho u_i u_j}, \quad (4.3.3.4)$$

and denote with f_{a-b} a value that is interpolated between values that are available for f_a and f_b . Referring to Fig. 3, we compute the terms that contribute to the FORTRAN symbol RSTU as follows:

Figure 3. Indexing of cells and nodes for computation of RSTU

$$AY_4 = A_{f,i+1/2,j+1/2,k} = [AFLUY(m_0) + AFLUY(m_2)]/2 = (AY_0 + AY_2)/2, \quad (4.3.3.5a)$$

$$AY_3 = A_{f,i+1/2,j-1/2,k} = [AFLUY(m_3) + AFLUY(m_{23})]/2 = (AY_3 + AY_{23})/2, \quad (4.3.3.5b)$$

$$AZ_6 = A_{f,i+1/2,j,k+1/2} = [AFLUZ(m_0) + AFLUZ(m_2)]/2 = (AZ_0 + AZ_2)/2, \quad (4.3.3.5c)$$

$$AZ_5 = A_{f,i+1/2,j,k-1/2} = [AFLUZ(m_5) + AFLUZ(m_{25})]/2 = (AZ_5 + AZ_{25})/2, \quad (4.3.3.5d)$$

$$AX_2 = A_{f,i+1,j,k} = AFLUX(m_2), \quad (4.3.3.5e)$$

$$AX_1 = A_{f,i,j,k} = AFLUX(m_0), \quad (4.3.3.5f)$$

$$RUUX2 = \langle \overline{\rho u_1 u_1} \rangle_{i+1,j,k} = \langle \overline{\rho u_1 u_1} \rangle_2, \quad (4.3.3.6a)$$

$$RUUX1 = \langle \overline{\rho u_1 u_1} \rangle_{i,j,k} = \langle \overline{\rho u_1 u_1} \rangle_0, \quad (4.3.3.6b)$$

$$RUUY4 = \langle \overline{\rho u_1 u_2} \rangle_{i+1/2,j+1/2,k} = \langle \overline{\rho u_1 u_2} \rangle_A = \langle f^{12} \rangle_A \quad (4.3.3.6c)$$

$$\begin{aligned} &= (f_{0-2}^{12} \Delta y_{j+1} + f_{4-24}^{12} \Delta y_j) \frac{1}{\Delta y_j + \Delta y_{j+1}} \\ &= \left(\frac{f_0^{12} \Delta x_{i+1} + f_2^{12} \Delta x_i}{\Delta x_i + \Delta x_{i+1}} \Delta y_{j+1} + \frac{f_4^{12} \Delta x_{i+1} + f_{24}^{12} \Delta x_i}{\Delta x_i + \Delta x_{i+1}} \Delta y_j \right) \frac{1}{\Delta y_j + \Delta y_{j+1}} \\ &= \frac{1}{(\Delta x_i + \Delta x_{i+1})(\Delta y_j + \Delta y_{j+1})} \left[(f_0^{12} \Delta x_{i+1} + f_2^{12} \Delta x_i) \Delta y_{j+1} + (f_4^{12} \Delta x_{i+1} + f_{24}^{12} \Delta x_i) \Delta y_j \right], \end{aligned}$$

$$RUUY3 = \langle \overline{\rho u_1 u_2} \rangle_{i+1/2,j-1/2,k} = \langle \overline{\rho u_1 u_2} \rangle_B = \langle f^{12} \rangle_B \quad (4.3.3.6d)$$

$$\begin{aligned} &= (f_{0-2}^{12} \Delta y_{j-1} + f_{3-23}^{12} \Delta y_j) \frac{1}{\Delta y_j + \Delta y_{j-1}} \\ &= \frac{1}{(\Delta x_i + \Delta x_{i+1})(\Delta y_j + \Delta y_{j-1})} \left[(f_0^{12} \Delta x_{i+1} + f_2^{12} \Delta x_i) \Delta y_{j-1} + (f_3^{12} \Delta x_{i+1} + f_{23}^{12} \Delta x_i) \Delta y_j \right], \end{aligned}$$

$$RUUZ6 = \langle \overline{\rho u_1 u_3} \rangle_{i+1/2,j,k+1/2} = \langle \overline{\rho u_1 u_3} \rangle_C = \langle f^{13} \rangle_C$$

$$= \langle f_{0-2}^{13} \Delta z_{k+1} + f_{6-26}^{13} \Delta z_k \rangle \frac{1}{\Delta z_k + \Delta z_{k+1}} \quad (4.3.3.6e)$$

$$= \frac{1}{(\Delta x_i + \Delta x_{i+1})(\Delta z_k + \Delta z_{k+1})} \left[(f_0^{13} \Delta x_{i+1} + f_2^{13} \Delta x_i) \Delta z_{k+1} + (f_6^{13} \Delta x_{i+1} + f_{26}^{13} \Delta x_i) \Delta z_k \right],$$

$$\begin{aligned}
RUUZ5 &= \langle \overline{\rho u_1 u_3} \rangle_{i+1/2, j, k-1/2} = \langle \overline{\rho u_1 u_3} \rangle_D = \langle f^{13} \rangle_D \\
&= \langle f_{0-2}^{13} \Delta z_{k-1} + f_{5-25}^{13} \Delta z_k \rangle \frac{1}{\Delta z_k + \Delta z_{k-1}} \\
&= \frac{1}{(\Delta x_1 + \Delta x_{i+1})(\Delta z_k + \Delta z_{k-1})} \left[(f_0^{13} \Delta x_{i+1} + f_2^{13} \Delta x_i) \Delta z_{k-1} + (f_5^{13} \Delta x_{i+1} + f_{25}^{13} \Delta x_i) \Delta z_k \right].
\end{aligned} \tag{4.3.3.6f}$$

Collecting all of the contributions we have

$$\begin{aligned}
RSTU &= -AX_2 \cdot RUUX2 + AX_1 \cdot RUUX1 - AY_4 \cdot RUUY4 + AY_3 \cdot RUUY3 \\
&\quad - AZ_6 \cdot RUUZ6 + AZ_5 \cdot RUUZ5.
\end{aligned} \tag{4.3.3.7}$$

Referring to Fig. 4, we compute the terms contributing to the FORTRAN symbol RSTV as follows:

$$AX_2 = A_{f,i+1/2,j+1/2,k} = [AFLUX(m_0) + AFLUX(m_4)]/2 = (AX_0 + AX_4)/2, \tag{4.3.3.8a}$$

$$AX_1 = A_{f,i-1/2,j+1/2,k} = [AFLUX(m_1) + AFLUX(m_{14})]/2 = (AX_1 + AX_{14})/2, \tag{4.3.3.8b}$$

$$AY_4 = A_{f,i,j+1,k} = AFLUY(m_4), \tag{4.3.3.8c}$$

$$AY_3 = A_{f,i,j,k} = AFLUY(m_0), \tag{4.3.3.8d}$$

$$AZ_6 = A_{f,i,j+1/2,k+1/2} = [AFLUZ(m_0) + AFLUZ(m_4)]/2 = (AZ_0 + AZ_4)/2, \tag{4.3.3.8e}$$

Figure 4. Indexing of cells and nodes for computation of RSTV

$$AZ_5 = A_{f,i,j+1/2,k-1/2} = [AFLUZ(m_5) + AFLUZ(m_{45})]/2 = (AZ_5 + AZ_{45})/2, \quad (4.3.3.8f)$$

$$RUUX2 = \langle \overline{\rho u_1 u_2} \rangle_{i+1/2,j+1/2,k} = \langle \overline{\rho u_1 u_2} \rangle_A = \langle f^{12} \rangle_A \quad (4.3.3.9a)$$

$$= \left(f_{0-4}^{12} \Delta x_{i+1} + f_{2-24}^{12} \Delta x_i \right) \frac{1}{\Delta x_i + \Delta x_{i+1}}$$

$$= \frac{1}{(\Delta x_i + \Delta x_{i+1})(\Delta y_j + \Delta y_{j+1})} \left[(f_0^{12} \Delta y_{j+1} + f_4^{12} \Delta y_j) \Delta x_{i+1} + (f_2^{12} \Delta y_{j+1} + f_{24}^{12} \Delta y_j) \Delta x_i \right],$$

$$RUUX1 = \langle \overline{\rho u_1 u_2} \rangle_{i-1/2,j+1/2,k} = \langle \overline{\rho u_1 u_2} \rangle_B = \langle f^{12} \rangle_B \quad (4.3.3.9b)$$

$$= \left(f_{0-4}^{12} \Delta x_{i-1} + f_{1-14}^{12} \Delta x_i \right) \frac{1}{\Delta x_i + \Delta x_{i-1}}$$

$$= \frac{1}{(\Delta x_i + \Delta x_{i-1})(\Delta y_j + \Delta y_{j+1})} \left[(f_0^{12} \Delta y_{j+1} + f_4^{12} \Delta y_j) \Delta x_{i-1} + (f_1^{12} \Delta y_{j+1} + f_{14}^{12} \Delta y_j) \Delta x_i \right],$$

$$RUUY4 = \langle \overline{\rho u_2 u_2} \rangle_{i,j+1,k} = \langle \overline{\rho u_2 u_2} \rangle_4, \quad (4.3.3.9c)$$

$$RUUY3 = \langle \overline{\rho u_2 u_2} \rangle_{i,j,k} = \langle \overline{\rho u_2 u_2} \rangle_0, \quad (4.3.3.9d)$$

$$RUUZ6 = \langle \overline{\rho u_2 u_3} \rangle_{i,j+1/2,k+1/2} = \langle \overline{\rho u_2 u_3} \rangle_C = \langle f^{23} \rangle_C$$

$$= \left(f_{0-4}^{23} \Delta z_{k+1} + f_{6-46}^{23} \Delta z_k \right) \frac{1}{\Delta z_k + \Delta z_{k+1}} \quad (4.3.3.9e)$$

$$= \frac{1}{(\Delta z_k + \Delta z_{k+1})(\Delta y_j + \Delta y_{j+1})} \left[(f_0^{23} \Delta y_{j+1} + f_4^{23} \Delta y_j) \Delta z_{k+1} + (f_6^{23} \Delta y_{j+1} + f_{46}^{23} \Delta y_j) \Delta z_k \right],$$

$$RUUZ5 = \langle \overline{\rho u_2 u_3} \rangle_{i,j+1/2,k-1/2} = \langle \overline{\rho u_2 u_3} \rangle_D = \langle f^{23} \rangle_D \quad (4.3.3.9f)$$

$$= \left(f_{0-4}^{23} \Delta z_{k-1} + f_{5-45}^{23} \Delta z_k \right) \frac{1}{\Delta z_k + \Delta z_{k-1}}$$

$$= \frac{1}{(\Delta z_k + \Delta z_{k-1})(\Delta y_j + \Delta y_{j+1})} \left[(f_0^{23} \Delta y_{j+1} + f_4^{23} \Delta y_j) \Delta z_{k-1} + (f_5^{23} \Delta y_{j+1} + f_{45}^{23} \Delta y_j) \Delta z_k \right].$$

Collecting all of the contributions, we have

$$RSTV = -AX_2 \cdot RUUX2 + AX_1 \cdot RUUX1 - AY_4 \cdot RUUY4 + AY_3 \cdot RUUY3$$

$$-AZ_6 \cdot RUUZ6 + AZ_5 \cdot RUUZ5. \quad (4.3.3.10)$$

Figure 5. Indexing of cells and nodes for computation of RSTW

Referring to Fig. 5, we compute the terms contributing to the FORTRAN symbol RSTW as follows:

$$AX2 = A_{f,i+1/2,j,k+1/2} = [AFLUX(m_0) + AFLUX(m_6)]/2 = (AX_0 + AX_6)/2, \quad (4.3.3.11.a)$$

$$AX1 = A_{f,i-1/2,j,k+1/2} = [AFLUX(m_1) + AFLUX(m_{16})]/2 = (AX_1 + AX_{16})/2, \quad (4.3.3.11.b)$$

$$AY4 = A_{f,i,j+1/2,k+1/2} = [AFLUY(m_0) + AFLUY(m_6)]/2 = (AY_0 + AY_6)/2, \quad (4.3.3.11.c)$$

$$AY3 = A_{f,i,j-1/2,k+1/2} = [AFLUY(m_3) + AFLUY(m_{36})]/2 = (AY_3 + AY_{36})/2, \quad (4.3.3.11.d)$$

$$AZ6 = A_{f,i,j-1/2,k+1} = AFLUZ(m_6), \quad (4.3.3.11.e)$$

$$AZ5 = A_{f,ijk} = AFLUZ(m_0), \quad (4.3.3.11.f)$$

$$RUUX2 = \langle \overline{\rho u_3 u_1} \rangle_{i+1/2,j,k+1/2} = \langle \overline{\rho u_3 u_1} \rangle_A = \langle f^{31} \rangle_A$$

$$= \left(f_{6-0}^{31} \Delta x_{i+1} + f_{2-26}^{31} \Delta x_i \right) \frac{1}{\Delta x_i + \Delta x_{i+1}} \quad (4.3.3.12.a)$$

$$= \left[\frac{(f_6^{31} \Delta z_k + f_0^{31} \Delta z_{k+1})}{(\Delta x_i + \Delta x_{i+1})(\Delta z_k + \Delta z_{k+1})} \Delta x_{i+1} + \frac{(f_{26}^{31} \Delta z_k + f_2^{31} \Delta z_{k+1})}{\Delta z_k + \Delta z_{k+1}} \Delta x_i \right]$$

$$= \frac{1}{(\Delta x_i + \Delta x_{i+1})(\Delta z_k + \Delta z_{k+1})} \left[(f_6^{31} \Delta z_k + f_0^{31} \Delta z_{k+1}) \Delta x_{i+1} + (f_{26}^{31} \Delta z_k + f_2^{31} \Delta z_{k+1}) \Delta x_i \right],$$

$$RUUX1 = \langle \overline{\rho u_3 u_1} \rangle_{i-1/2,j,k+1/2} = \langle \overline{\rho u_3 u_1} \rangle_B = \langle f^{31} \rangle_B \quad (4.3.3.12.b)$$

$$\begin{aligned}
&= \left(f_{6-0}^{31} \Delta x_{i-1} + f_{16-1}^{31} \Delta x_i \right) \frac{1}{\Delta x_i + \Delta x_{i-1}} \\
&= \frac{1}{(\Delta x_i + \Delta x_{i-1})(\Delta z_k + \Delta z_{k+1})} \left[\left(f_6^{31} \Delta z_k + f_0^{31} \Delta z_{k+1} \right) \Delta x_{i-1} + \left(f_{16}^{31} \Delta z_k + f_1^{31} \Delta z_{k+1} \right) \Delta x_i \right], \\
\text{RUUY4} &= \langle \overline{\rho u_3 u_2} \rangle_{i,j+1/2,k+1/2} = \langle \overline{\rho u_3 u_2} \rangle_C = \langle f^{32} \rangle_C \\
&= \left[f_{0-6}^{32} \Delta y_{j+1} + f_{46-4}^{32} \Delta y_j \right] \frac{1}{\Delta y_j + \Delta y_{j+1}} \quad (4.3.3.12c) \\
&= \frac{1}{(\Delta y_j + \Delta y_{j+1})(\Delta z_k + \Delta z_{k+1})} \left[\left(f_6^{32} \Delta z_k + f_0^{32} \Delta z_{k+1} \right) \Delta y_{j+1} + \left(f_{46}^{32} \Delta z_k + f_4^{32} \Delta z_{k+1} \right) \Delta y_j \right], \\
\text{RUUY3} &= \langle \overline{\rho u_3 u_2} \rangle_{i,j-1/2,k+1/2} = \langle \overline{\rho u_3 u_2} \rangle_D = \langle f^{32} \rangle_D \\
&= \left[f_{0-6}^{32} \Delta y_{j-1} + f_{3-36}^{32} \Delta y_j \right] \frac{1}{\Delta y_j + \Delta y_{j-1}} \\
&= \frac{1}{(\Delta y_j + \Delta y_{j-1})(\Delta z_k + \Delta z_{k+1})} \left[\left(f_6^{32} \Delta z_k + f_0^{32} \Delta z_{k+1} \right) \Delta y_{j-1} + \left(f_{36}^{32} \Delta z_k + f_3^{32} \Delta z_{k+1} \right) \Delta y_j \right], \quad (4.3.3.12d)
\end{aligned}$$

$$\text{RUUZ6} = \langle \overline{\rho u_3 u_3} \rangle_{i,j,k+1} = \langle \overline{\rho u_3 u_3} \rangle_6, \quad (4.3.3.12e)$$

$$\text{RUUZ5} = \langle \overline{\rho u_3 u_3} \rangle_{i,j,k} = \langle \overline{\rho u_3 u_3} \rangle_0. \quad (4.3.3.12f)$$

Collecting all of the contributions, we have

$$\begin{aligned}
\text{RSTW} &= -\text{AX2} \cdot \text{RUUX2} + \text{AX1} \cdot \text{RUXX1} - \text{AY4} \cdot \text{RUUY4} + \text{AY3} \cdot \text{RUUY3} \\
&\quad - \text{AZ6} \cdot \text{RUUZ6} + \text{AZ5} \cdot \text{RUUZ5}. \quad (4.3.3.13)
\end{aligned}$$

4.3.4 Computation of Turbulent Fluxes, Implicit Formulation

Equation 4.3.1.1 can be rewritten as

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j U_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[(\mu_\ell + \mu_t^{ij}) \right] \frac{\partial U_i}{\partial x_j} + \rho g_i - R_i \quad (4.3.4.1)$$

with

$$\mu^{ij} = \bar{\mu}_t : \bar{\delta}_i \bar{\delta}_j = \frac{-\overline{\rho u_i u_j}}{\partial U_i / \partial X_j} \quad (4.3.4.2)$$

and

$$\bar{\mu}_t = \left(-\frac{\overline{\rho u_\ell u_m}}{\partial U_\ell / \partial X_m} \right) \bar{\delta}_\ell \bar{\delta}_m = \mu_{\ell m} \bar{\delta}_\ell \bar{\delta}_m. \quad (4.3.4.3)$$

The effective turbulent viscosity $\bar{\mu}_t$ now has a tensor character and Eq. 4.3.1.4 for the diffusive turbulent flux is replaced by

$$J_{mij}^{dt} = -\mu_t^{ij} \frac{\partial U_i}{\partial X_j}. \quad (4.3.4.4)$$

Thus, formally, the laminar and turbulent diffusive fluxes can be treated numerically in the same way. Equation 4.3.2.4 for the discretized turbulent fluxes is replaced by

$$\left\langle J_{m\alpha}^{dt} A_f \right\rangle_{\alpha+1/2}^{n+1} = - \left\langle \mu_t^{ij} \frac{\partial U_i}{\partial X_\alpha} A_f \right\rangle_{\alpha+1/2} = -D_{\alpha+1/2}^{mt} (U_{i,\alpha+1}^{n+1} - U_{i,\alpha}^{n+1}), \quad (4.3.4.5a)$$

$$\left\langle J_{m\alpha}^{dt} A_f \right\rangle_{\alpha-1/2}^{n+1} = - \left\langle \mu_t^{ij} \frac{\partial U_i}{\partial X_\alpha} A_f \right\rangle_{\alpha-1/2} = -D_{\alpha-1/2}^{mt} (U_{i,\alpha}^{n+1} - U_{i,\alpha-1}^{n+1}), \quad (4.3.4.5b)$$

with

$$D_{\alpha+1/2}^{mt} = \frac{A_{f,\alpha+1/2}}{\frac{1}{2} \left(\frac{\Delta X_\alpha}{\mu_t^{i\alpha}} + \frac{\Delta X_{\alpha+1}}{\mu_t^{i,\alpha+1}} \right)} \quad (4.3.4.6a)$$

and

$$D_{\alpha-1/2}^{mt} = \frac{A_{f,\alpha-1/2}}{\frac{1}{2} \left(\frac{\Delta X_\alpha}{\mu_t^{i\alpha}} + \frac{\Delta X_{\alpha-1}}{\mu_t^{i,\alpha-1}} \right)}. \quad (4.3.4.6b)$$

Formally, similar definitions hold for $D^{m\ell}$, replacing μ_t with μ_ℓ . The numerical treatment of the discretization of Eq. 4.3.4.1 follows the same pattern as that of Eq. 4.3.1.1, except that the laminar and turbulent diffusion terms are treated the same way. The final discretized momentum equation, which replaces Eq. 4.3.1.8, is

$$U_{io}^{n+1} \left\{ V_{fo} \frac{\rho_0^n}{\Delta t} + V_{fo} \frac{<R_i>_3}{U_{io}^n} + [0, F_{\alpha+1/2}] + [0, -F_{\alpha-1/2}] + D_{\alpha+1/2}^{m\ell} + D_{\alpha+1/2}^{mt} + D_{\alpha-1/2}^{m\ell} + D_{\alpha-1/2}^{mt} \right\} \\ - U_{i,\alpha+1}^{n+1} \left\{ [0, -F_{\alpha+1/2}] + D_{\alpha+1/2}^{m\ell} + D_{\alpha+1/2}^{mt} \right\} \quad (4.3.4.7)$$

$$\begin{aligned}
& - U_{i,\alpha-1}^{n+1} \left\{ [0, F_{\alpha-1/2}] + D_{\alpha-1/2}^{m\ell} + D_{\alpha-1/2}^{mt} \right\} + d_{i+1/2}^i (p_{i+1}^{n+1} - p_o^{n+1}) \\
& = V_{fo} \rho_o^n \frac{U_{io}^n}{\Delta t} - V_{fo} U_{io}^n \left(\frac{\partial p}{\partial t} \right)_o^n + V_{fo} \langle \rho g_i \rangle_3.
\end{aligned}$$

Two code versions have been written. The first version uses the explicit formulation of the turbulent diffusion coefficients; the second, the implicit formulation. Although, theoretically, the implicit formulation should be better because it does not impose any constraint on the time step, in practice, it presents difficulty of convergence when the velocity gradients $\partial U_i / \partial x_j$, which appear in the definition of μ_t^{ij} , become locally very small.

4.4 Enthalpy Equation

4.4.1 Analytical Treatment

The transport equation that describes the space and time distribution of the enthalpy in the computational domain is

$$\rho \frac{\partial h}{\partial t} + \rho U_j \frac{\partial h}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} - \rho c_p \overline{u_j \phi} \right) + S_h. \quad (4.4.1.1)$$

In this case, contrary to the $k-\epsilon$ turbulence model, the term that describes the turbulent diffusion $-\rho c_p \overline{u_j \phi}$ is not modeled as a function of the enthalpy gradients, but retains its theoretical rigorous formulation. S_h represents a power source.

Using the discretized form of the continuity equation 3.1.41, we can rewrite Eq. 4.4.1.1 as

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j h) = \frac{\partial}{\partial x_j} \left(\frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} - \rho c_p \overline{u_j \phi} \right) + S_h. \quad (4.4.1.2)$$

If we define convective, diffusive (laminar and turbulent), and total (convective plus diffusive) enthalpy fluxes as

$$J_{hj}^c = \rho U_j h, \quad (4.4.1.3)$$

$$J_{hj}^{d\ell} = - \frac{\lambda}{c_p} \frac{\partial h}{\partial x_j}, \quad (4.4.1.4)$$

$$J_{hj}^{dt} = \rho c_p \overline{u_j \phi}, \quad (4.4.1.5)$$

and

$$J_{hj} = \rho U_j h - \frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} + \rho c_p \overline{u_j \phi} = J_{hj}^c + J_{hj}^{d\ell} + J_{hj}^{dt}, \quad (4.4.1.6)$$

we can rewrite Eq. 4.4.1.2 in the compact form

$$\frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_j} J_{hi} = S_h. \quad (4.4.1.7)$$

Integration of Eq. 4.4.1.7 over the volume V_f and application of the Gauss theorem yields

$$\begin{aligned} \int_{V_f} \frac{\partial(\rho h)}{\partial t} dV + \int_{A_{f,i+1/2}} J_{hi} dA - \int_{A_{f,i-1/2}} J_{hi} dA + \int_{A_{f,j+1/2}} J_{hj} dA - \int_{A_{f,j-1/2}} J_{hj} dA \\ + \int_{A_{f,k+1/2}} J_{hk} dA - \int_{A_{f,k-1/2}} J_{hk} dA = \int_{V_f} S_h dV. \end{aligned} \quad (4.4.1.8)$$

4.4.2 Numerical Treatment

Equation 4.4.1.8 is discretized as follows:

$$\begin{aligned} \frac{V_{fo}}{\Delta t} [(\rho h)_o^{n+1} - (\rho h)_o^n] + \langle J_h^c A_f \rangle_{\alpha+1/2}^{n+1} - \langle J_h^c A_f \rangle_{\alpha-1/2}^{n+1} \\ + \langle (J_h^{d\ell} + J_h^{dt}) A_f \rangle_{\alpha+1/2}^{n+1} - \langle (J_h^{d\ell} + J_h^{dt}) A_f \rangle_{\alpha-1/2}^{n+1} = V_f \langle S_h \rangle_3^{n+1}, \end{aligned} \quad (4.4.2.1)$$

where summation for $\alpha = i, j, k$ is implied.

The convective fluxes are computed as follows:

$$\langle J_h^c A_f \rangle_{\alpha+1/2}^{n+1} = \langle \rho U h A_f \rangle_{\alpha+1/2}^{n+1} = \langle F h \rangle_{\alpha+1/2}^{n+1} = [0, F_{\alpha+1/2}] h_{\alpha}^{n+1} - [0, -F_{\alpha+1/2}] h_{\alpha+1}^{n+1}, \quad (4.4.2.2a)$$

$$\langle J_h^c A_f \rangle_{\alpha-1/2}^{n+1} = [0, F_{\alpha-1/2}] h_{\alpha-1}^{n+1} - [0, -F_{\alpha-1/2}] h_{\alpha}^{n+1}. \quad (4.4.2.2b)$$

The laminar diffusive fluxes are computed, with $\Gamma_h = \lambda / c_p$, by

$$\langle J_h^{d\ell} A_f \rangle_{\alpha+1/2}^{n+1} = - \left\langle \Gamma_h \frac{\partial h}{\partial x_{\alpha}} A_f \right\rangle_{\alpha+1/2}^{n+1} = - \frac{A_{f,\alpha+1/2} (h_{\alpha+1} - h_{\alpha})^{n+1}}{\frac{1}{2} \left(\frac{\Delta x_{\alpha}}{\Gamma_{h,\alpha}} + \frac{\Delta x_{\alpha+1}}{\Gamma_{h,\alpha+1}} \right)} = - D_{\alpha+1/2}^h (h_{\alpha+1} - h_{\alpha})^{n+1}, \quad (4.4.2.3a)$$

$$\langle J_h^{d\ell} A_f \rangle_{\alpha-1/2}^{n+1} = - \left\langle \Gamma_h \frac{\partial h}{\partial x_{\alpha}} A_f \right\rangle_{\alpha-1/2}^{n+1} = - \frac{A_{f,\alpha-1/2} (h_{\alpha} - h_{\alpha-1})^{n+1}}{\frac{1}{2} \left(\frac{\Delta x_{\alpha-1}}{\Gamma_{h,\alpha-1}} + \frac{\Delta x_{\alpha}}{\Gamma_{h,\alpha}} \right)} = - D_{\alpha-1/2}^h (h_{\alpha} - h_{\alpha-1})^{n+1}.$$

(4.4.2.3b)

The definition of the diffusion coefficients is formally identical with that of Eq. 3.1.36. The terms for the turbulent diffusion are computed by

$$\langle J_h^{dt} A_f \rangle_{\alpha+1/2}^{n+1} = \langle \rho c_p \overline{u_\alpha \phi} A_f \rangle_{\alpha+1/2}^{n+1} = A_{f,\alpha+1/2} \frac{(\rho c_p \overline{u_\alpha \phi})_{\alpha+1/2}^{n+1} \Delta x_\alpha + (\rho c_p \overline{u_\alpha \phi})_\alpha^{n+1} \Delta x_{\alpha+1}}{\Delta x_\alpha + \Delta x_{\alpha+1}}, \quad (4.4.2.4a)$$

$$\langle J_h^{dt} A_f \rangle_{\alpha-1/2}^{n+1} = \langle \rho c_p \overline{u_\alpha \phi} A_f \rangle_{\alpha-1/2}^{n+1} = A_{f,\alpha-1/2} \frac{(\rho c_p \overline{u_\alpha \phi})_\alpha^{n+1} \Delta x_{\alpha-1} + (\rho c_p \overline{u_\alpha \phi})_{\alpha-1}^{n+1} \Delta x_\alpha}{\Delta x_\alpha + \Delta x_{\alpha-1}}. \quad (4.4.2.4b)$$

Inserting Eqs. 4.4.2.2-4.4.2.4 into Eq. 4.4.2.1, we obtain

$$\begin{aligned} & \frac{V_{fo}}{\Delta t} \left[(\rho h)_0^{n+1} - (\rho h)_0^n \right] + [0, F_{\alpha+1/2}] h_\alpha^{n+1} - [0, -F_{\alpha+1/2}] h_{\alpha+1}^{n+1} \\ & - [0, F_{\alpha-1/2}] h_{\alpha-1}^{n+1} + [0, -F_{\alpha-1/2}] h_\alpha^{n+1} - D_{\alpha+1/2}^h (h_{\alpha+1} - h_\alpha)^{n+1} + D_{\alpha-1/2}^h (h_\alpha - h_{\alpha-1})^{n+1} \\ & + A_{f,\alpha+1/2} \frac{(\rho c_p \overline{u_\alpha \phi})_{\alpha+1}^{n+1} \Delta x_\alpha + (\rho c_p \overline{u_\alpha \phi})_\alpha^{n+1} \Delta x_{\alpha+1}}{\Delta x_\alpha + \Delta x_{\alpha+1}} \\ & - A_{f,\alpha-1/2} \frac{(\rho c_p \overline{u_\alpha \phi})_\alpha^{n+1} \Delta x_{\alpha-1} + (\rho c_p \overline{u_\alpha \phi})_{\alpha-1}^{n+1} \Delta x_\alpha}{\Delta x_\alpha + \Delta x_{\alpha-1}} = V_{fo} \langle S_h \rangle_3^{n+1}. \end{aligned} \quad (4.4.2.5)$$

The discretized terms for the turbulent diffusion are treated numerically as a contribution to the source term, i.e., by bringing them to the right-hand side of the equation. Rearranging Eq. 4.4.2.5, we obtain

$$\begin{aligned} & h_0^{n+1} \left\{ \frac{V_{go} \rho_0^{n+1}}{\Delta t} + [0, F_{\alpha+1/2}] + [0, -F_{\alpha-1/2}] + D_{\alpha+1/2}^h + D_{\alpha-1/2}^h \right\} \\ & - h_{\alpha+1}^{n+1} \left\{ [0, -F_{\alpha+1/2}] + D_{\alpha+1/2}^h \right\} - h_{\alpha-1}^{n+1} \left\{ [0, F_{\alpha-1/2}] + D_{\alpha-1/2}^h \right\} \\ & = V_{fo} \frac{(\rho h)_0^n}{\Delta t} + V_{fo} \langle S_h \rangle_3^{n+1} - A_{f,\alpha+1/2} \frac{(\rho c_p \overline{u_\alpha \phi})_{\alpha+1}^{n+1} \Delta x_\alpha + (\rho c_p \overline{u_\alpha \phi})_\alpha^{n+1} \Delta x_{\alpha+1}}{\Delta x_\alpha + \Delta x_{\alpha+1}} \\ & + A_{f,\alpha-1/2} \frac{(\rho c_p \overline{u_\alpha \phi})_\alpha^{n+1} \Delta x_{\alpha-1} + (\rho c_p \overline{u_\alpha \phi})_{\alpha-1}^{n+1} \Delta x_\alpha}{\Delta x_\alpha + \Delta x_{\alpha-1}}. \end{aligned} \quad (4.4.2.6)$$

Equation 4.4.2.6 can be written in the compact form

$$\alpha_o^h h_o^{n+1} - \sum_{\beta=1}^6 \beta a_{\beta}^h h_{\beta}^{n+1} = b_o^h, \quad (4.4.2.7)$$

with the following definitions for the coefficients:

$$a_o^h = \frac{V_{fo} \rho_o^{n+1}}{\Delta t} + [0, F_{\alpha+1/2}] + [0, -F_{\alpha-1/2}] + D_{\alpha+1/2}^h + D_{\alpha-1/2}^h \quad (\alpha = i, j, k), \quad (4.4.2.8a)$$

$$a_1^h = [0, F_{i-1/2}] + D_{i-1/2}^h, \quad (4.4.2.8b)$$

$$a_2^h = [0, -F_{i+1/2}] + D_{i+1/2}^h, \quad (4.4.2.8c)$$

$$a_3^h = [0, F_{j-1/2}] + D_{j-1/2}^h, \quad (4.4.2.8d)$$

$$a_4^h = [0, -F_{j+1/2}] + D_{j+1/2}^h, \quad (4.4.2.8e)$$

$$a_5^h = [0, F_{k-1/2}] + D_{k-1/2}^h, \quad (4.4.2.8f)$$

$$a_6^h = [0, -F_{k+1/2}] + D_{k+1/2}^h, \quad (4.4.2.8g)$$

$$b_o^h = \frac{V_{fo}}{\Delta t} (\rho h)_o^n + V_{fo} \langle S_h \rangle_3^{n+1} + A_{f,\alpha+1/2} \frac{(\rho c_p \overline{u_{\alpha} \phi})_{\alpha+1}^{n+1} \Delta x_{\alpha} + (\rho c_p \overline{u_{\alpha} \phi})_{\alpha}^{n+1} \Delta x_{\alpha+1}}{\Delta x_{\alpha} + \Delta x_{\alpha+1}} \quad (4.4.2.8h)$$

$$- A_{f,\alpha-1/2} \frac{(\rho c_p \overline{u_{\alpha} \phi})_{\alpha}^{n+1} \Delta x_{\alpha-1} + (\rho c_p \overline{u_{\alpha} \phi})_{\alpha-1}^{n+1} \Delta x_{\alpha}}{\Delta x_{\alpha} + \Delta x_{\alpha-1}}.$$

Again, using the discretized continuity Eq. 3.1.41, we obtain the second form of the coefficient a_o :

$$a_o^{lh} = \frac{V_{fo}}{\Delta t} \rho_o^n + [0, F_{\alpha-1/2}] + [0, -F_{\alpha+1/2}] + D_{\alpha+1/2}^h + D_{\alpha-1/2}^h \quad (\alpha = i, j, k). \quad (4.4.2.9)$$

5 Synopsis of Governing Equations

For reference, the transport equations used for the RSM, including the relative momentum and enthalpy equations, are summarized in Table I.

Table I. Summary of transport equations used for
Reynolds stress model of turbulence

1. Scalar fluxes

Rigorous

$$\frac{\partial(\overline{u_i\phi})}{\partial t} + U_j \frac{\partial(\overline{u_i\phi})}{\partial x_j} = -\frac{\partial}{\partial x_j} \left(\overline{u_i u_j \phi} + \frac{1}{\rho} \overline{p \phi} \delta_{ij} \right) - \left(\overline{u_i u_j} \frac{\partial T}{\partial x_j} + \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} \right) - \beta g_i \overline{\phi^2} + \frac{1}{\rho} \overline{p} \frac{\partial \phi}{\partial x_i} \quad (3.1.1)$$

Modeled

$$\frac{\partial(\overline{u_i\phi})}{\partial t} + \frac{\partial}{\partial x_j} \left[U_j (\overline{u_i\phi}) - \Gamma_\phi^v \frac{\partial(\overline{u_i\phi})}{\partial x_j} \right] = P_{i\phi} + G_{i\phi} (1 - c_{3\phi}) - c_{1\phi} \frac{\varepsilon}{k} \overline{u_i\phi} + c_{2\phi} \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} + \pi_{i\phi}^w \quad (3.1.16)$$

2. Variance of temperature fluctuations

Rigorous

$$\frac{\partial \overline{\phi^2}}{\partial t} + U_j \frac{\partial \overline{\phi^2}}{\partial x_j} = -\frac{\partial}{\partial x_j} (\overline{u_j \phi^2}) + \frac{\partial}{\partial x_j} \left(\frac{\lambda}{\rho c_p} \frac{\partial \overline{\phi^2}}{\partial x_j} \right) - 2 \overline{u_j \phi} \frac{\partial T}{\partial x_j} - 2 \frac{\lambda}{\rho c_p} \frac{\partial \phi}{\partial x_j} \frac{\partial \phi}{\partial x_j} \quad (3.2.1)$$

Modeled

$$\frac{\partial \overline{g}}{\partial t} + \frac{\partial(\overline{U_j g})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(c_\phi \frac{k^2}{\varepsilon} \frac{\partial \overline{g}}{\partial x_j} + \frac{\lambda}{\rho c_p} \frac{\partial \overline{g}}{\partial x_j} \right) - \overline{u_j \phi} \frac{\partial T}{\partial x_j} - \frac{\varepsilon}{k} \frac{\overline{g}}{R} \quad (3.2.8)$$

3. Reynolds stresses

Rigorous

$$\frac{\partial \overline{u_i u_j}}{\partial t} + U_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} = -\frac{\partial}{\partial x_\ell} (\overline{u_\ell u_i u_j}) - \frac{1}{\rho} \left(\frac{\partial \overline{u_j p}}{\partial x_i} + \frac{\partial \overline{u_i p}}{\partial x_j} \right) + P_{ij} + G_{ij} + \pi_{ij} - \varepsilon_{ij} \quad (4.1.1.1)$$

Modeled

$$\frac{\partial \overline{u_i u_j}}{\partial t} + U_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} = \frac{\partial}{\partial x_\ell} \left(\nu_\ell \frac{\partial \overline{u_i u_j}}{\partial x_\ell} + c_s \frac{k^2}{\varepsilon} \frac{\partial \overline{u_i u_j}}{\partial x_\ell} \right) - (1 - c_2) \left(\overline{u_i u_\ell} \frac{\partial U_j}{\partial x_\ell} + \overline{u_j u_\ell} \frac{\partial U_i}{\partial x_\ell} \right)$$

Table I. (Continued)

$$\begin{aligned}
& - (1 - c_3)(\beta g_i \overline{u_j \phi} + \beta g_j \overline{u_i \phi}) - c_1 \frac{\epsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) \\
& - c_2 \frac{2}{3} \overline{u_n u_m} \frac{\partial U_n}{\partial x_m} \delta_{ij} - c_3 \frac{2}{3} \beta g_\ell \overline{u_\ell \phi} \delta_{ij} + \pi_{ij}^w - \frac{2}{3} \epsilon \delta_{ij}. \quad (4.1.1.19)
\end{aligned}$$

4. Dissipation of turbulent kinetic energy

$$\rho \frac{\partial(\rho \epsilon)}{\partial t} + \rho U_j \frac{\partial \epsilon}{\partial x_j} = c_{13} \frac{\epsilon}{k} (P_k + G_k)(1 + c_{3\epsilon} R_f) - c_{2\epsilon} \rho \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left(\mu_\ell \frac{\partial \epsilon}{\partial x_j} + c_\epsilon \rho \frac{k}{\epsilon} \overline{u_j u_m} \frac{\partial \epsilon}{\partial x_m} \right) \quad (4.2.1.1)$$

5. Momentum

$$\frac{\partial(\rho U_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j U_i) = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu_\ell \frac{\partial U_i}{\partial x_j} - \rho \overline{u_i u_j} \right) + \rho g_i = R_i \quad (4.3.1.1)$$

6. Enthalpy

$$\rho \frac{\partial h}{\partial t} + \rho U_j \frac{\partial h}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\lambda}{c_p} \frac{\partial h}{\partial x_j} - \rho c_p \overline{u_j \phi} \right) + S_h \quad (4.4.1.1)$$

All of the constants that are used in the governing equations are summarized in Table II.

All of the transport equations have been reduced to the generalized form

$$\frac{\partial \Phi}{\partial t} + \frac{\partial J_{\Phi i}}{\partial x_j} = S_\Phi, \quad (5.1)$$

with proper definitions of the transported quantity Φ , of the flux J_Φ , and of the source term S_Φ . These definitions are summarized in Table III.

Table II. Summary of constants used in 11-equation Reynolds stress model

Transport Equation	Symbols of Transported Quantity	Constants
Scalar fluxes	$\overline{u_i \phi}$	$\sigma_\phi = 1.3$ $c_\mu = 0.09$ $c_{s\phi} = c_\mu / \sigma_\phi = 0.07$ $c_{1\phi} = 3.1$ $c_{2\phi} = 0.4$ $c_{3\phi} = 0.5$ $c'_{1\phi} = 0.5$ $\sigma_t = 0.9$
Variance of temperature fluctuation	$g = \overline{\phi^2} / 2$	$c_\phi = 0.13$ $R = 0.5$ $A^+ = 0.025$ $c_g = 1.0$
Reynolds stresses	$\overline{u_i u_j}$	$c_s = 0.09$ $c_1 = 2.8$ $c_2 = 0.47$ $c_3 = 0.47$ $E = 9.0$
Dissipation of turbulent kinetic energy	ε	$c_{1\varepsilon} = 1.44$ $c_{2\varepsilon} = 1.92$ $c_{3\varepsilon} = 0.8$ $c_\varepsilon = 0.15$

Table III. Definitions of transported quantity Φ , flux J_Φ , and source term S_Φ of generalized transport equation $\frac{\partial \Phi}{\partial t} + \frac{\partial J_\Phi}{\partial x_j} = S_\Phi$, for governing equations of Reynolds stress model

Equation	Transported Quantity Φ	Flux J_Φ	Source S_Φ
Scalar fluxes	$\Phi_i = \rho \overline{u_i \phi}$	$J_{\Phi ij} = \rho U_j (\overline{u_i \phi}) - \rho \left(\nu_\ell + c_{s\phi} \frac{k^2}{\varepsilon} \right) \frac{\partial \overline{u_i \phi}}{\partial x_j}$	$S_{\Phi i} = \rho \left[P_{i\phi} + G_{i\phi} (1 - c_{3\phi}) - c_{1\phi} \frac{\varepsilon}{k} \overline{u_i \phi} + c_{2\phi} \overline{u_j \phi} \frac{\partial U_i}{\partial x_j} + \pi_{i\phi}^w \right]$
Variance of temperature fluctuations	$\Phi_g = g = \frac{1}{2} \overline{\phi^2}$	$J_g = U_{ig} - \left(\frac{\lambda}{\rho c_p} + c_\phi \frac{k^2}{\varepsilon} \right) \frac{\partial g}{\partial x_i}$	$S_g = P_g - \varepsilon g$
Reynolds stresses	$\Phi_{ij} = \overline{u_i u_j}$	$J_\ell(\Phi_{ij}) = U_\ell \overline{u_i u_j} - \left(\nu_\ell + c_s \frac{k^2}{\varepsilon} \right) \frac{\partial \overline{u_i u_j}}{\partial x_\ell}$	$S_{\Phi ij} = -(1 - c_2) \left(\overline{u_i u_\ell} \frac{\partial U_j}{\partial x_\ell} + \overline{u_j u_\ell} \frac{\partial U_i}{\partial x_\ell} \right) - (1 - c_3) \left(\beta g_i \overline{u_j \phi} + \beta g_j \overline{u_i \phi} \right) - c_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) - c_2 \frac{2}{3} \frac{\overline{u_n u_m}}{\partial x_m} \frac{\partial U_n}{\partial x_m} \delta_{ij} - c_3 \frac{2}{3} \beta g_\ell \overline{u_\ell \phi} \delta_{ij} + \pi_{ij}^w - \frac{2}{3} \varepsilon \delta_{ij}$
Dissipation of turbulent kinetic energy	$\Phi_\varepsilon = \rho \varepsilon$	$J_{\varepsilon j} = \rho U_j \varepsilon - \mu_\ell \frac{\partial \varepsilon}{\partial x_j} - c_\varepsilon \rho \frac{k}{\varepsilon} \overline{u_i u_m} \frac{\partial \varepsilon}{\partial x_m}$	$S_\varepsilon = c_{1\varepsilon} \frac{\varepsilon}{k} (P_k + G_k) (1 + c_{3\varepsilon} R_f) - c_{2\varepsilon} \rho \frac{\varepsilon^2}{k}$
Momentum	$\Phi_i = \rho U_i$	$J_{mij} = \rho U_j U_i - \mu_\ell \frac{\partial U_i}{\partial x_j} + \overline{\rho u_i u_j}$	$S_{mi} = \rho g_i - \frac{\partial p}{\partial x_i} - R_i$
Enthalpy	$\Phi = \rho h$	$J_{hi} = \rho U_i h - \frac{\lambda}{c_p} \frac{\partial h}{\partial x_i} + \overline{\rho c_p u_i \phi}$	S_h

6 Validation of Reynolds Stress Model with Simulation of Homogeneous Turbulence

6.1 Reynolds Equations for Homogeneous Turbulence

The condition of homogeneity in turbulence requires an infinite spatial field that can be simulated numerically by a finite domain with slip-free boundary conditions. Early experiments on nearly homogeneous turbulence have been performed in wind tunnels with an almost unilateral flow with a constant velocity gradient. Turbulence generated by grids at the tunnel entrance becomes almost homogeneous in the center of the tunnel at some distance from the inlet. Among the most accurate and best documented experiments on homogeneous turbulence are those by Champagne et al.,¹⁸ which we chose as a benchmark for validating numerical computations.

The conditions that must be realized in a homogeneous turbulent shear flow are as follows. With reference to the sketch shown in Fig. 6, let x_1 be a coordinate along the horizontal axis of the wind tunnel and x_2 and x_3 be coordinates along the vertical and transverse axis of the tunnel, respectively. In homogeneous turbulence, the mean velocity components of the flow satisfy the conditions

$$U_1 = U_1(x_2) \quad (6.1.1a)$$

$$U_2 = U_3 = 0 \quad (6.1.1b)$$

$$\partial U_1 / \partial x_2 = \text{constant} \quad (6.1.1c)$$

$$\partial U_i / \partial x_j = 0 \quad (i, j) \neq (1, 2) \quad (6.1.1d)$$

Figure 6. Sketch of homogeneous shear flow

Let H be the height of the wind tunnel and $U_c = U_1 (H/2)$ be the center velocity. Under the conditions described in Eq. 6.1.1, the components of the stress production tensor become

$$P_{11} = -2\overline{u_1 u_2} \frac{\partial U_1}{\partial x_2}, \quad (6.1.2a)$$

$$P_{22} = 0, \quad (6.1.2b)$$

$$P_{33} = 0, \quad (6.1.2c)$$

$$P_{12} = -\overline{u_2 u_2} \frac{\partial U_1}{\partial x_2}, \quad (6.1.2d)$$

$$P_{13} = -\overline{u_2 u_3} \frac{\partial U_1}{\partial x_2}, \quad (6.1.2e)$$

$$P_{23} = 0. \quad (6.1.2f)$$

The Reynolds stress equations simplify to the following system of ordinary differential equations of the first order:

$$\frac{\partial}{\partial t} (\overline{u_1 u_2}) = P_{11} + \pi_{11} - \epsilon_{11} = -2\overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} + 2 \frac{\overline{p u_1}}{\rho \partial x_1} - 2\nu \frac{\partial u_1}{\partial x_\ell} \frac{\partial u_1}{\partial x_\ell}, \quad (6.1.3a)$$

$$\frac{\partial}{\partial t} (\overline{u_2 u_2}) = \pi_{22} - \epsilon_{22} = \frac{2\overline{p u_2}}{\rho \partial x_2} - 2\nu \frac{\partial u_2}{\partial x_\ell} \frac{\partial u_2}{\partial x_\ell}, \quad (6.1.3b)$$

$$\frac{\partial}{\partial t} (\overline{u_3 u_3}) = \pi_{33} - \epsilon_{33} = \frac{2\overline{p u_3}}{\rho \partial x_3} - 2\nu \frac{\partial u_3}{\partial x_\ell} \frac{\partial u_3}{\partial x_\ell}, \quad (6.1.3c)$$

$$\frac{\partial (\overline{u_1 u_2})}{\partial t} = P_{12} + \pi_{12} - \epsilon_{12} = -\overline{u_2 u_2} \frac{\partial U_1}{\partial x_2} + \frac{\overline{p \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right)}}{\rho} - 2\nu \frac{\partial u_1}{\partial x_\ell} \frac{\partial u_2}{\partial x_\ell}, \quad (6.1.3d)$$

$$\frac{\partial (\overline{u_1 u_3})}{\partial t} = P_{13} + \pi_{13} - \epsilon_{13} = -\overline{u_2 u_3} \frac{\partial U_1}{\partial x_2} + \frac{\overline{p \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right)}}{\rho} - 2\nu \frac{\partial u_1}{\partial x_\ell} \frac{\partial u_3}{\partial x_\ell}, \quad (6.1.3e)$$

$$\frac{\partial (\overline{u_2 u_3})}{\partial t} = \pi_{23} - \epsilon_{23} = \frac{\overline{p \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right)}}{\rho} - 2\nu \frac{\partial u_2}{\partial x_\ell} \frac{\partial u_3}{\partial x_\ell}. \quad (6.1.3f)$$

Summing Eqs. 6.1.3a-6.1.3c and taking into account $\pi_{ii} = 0$ (summation implied) and

$$P = \frac{P_{ii}}{2} = \frac{P_{11}}{2} = -\overline{u_1 u_2} \frac{\partial U_1}{\partial x_2}, \quad (6.1.4)$$

we obtain

$$\frac{\partial k}{\partial t} = P - \varepsilon = -\overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - \overline{v \frac{\partial u_1}{\partial x_\ell} \frac{\partial u_1}{\partial x_\ell}} \quad (6.1.5)$$

6.2 Reynolds Equations for Homogeneous Isotropic Turbulence

Several experimental results are given for the case of homogeneous isotropic turbulence. Therefore, for the validation of numerical computations, it is useful to consider how the above equations are modified under the assumption of local isotropy in the dissipation spectral range. The assumption of isotropic turbulence implies that

$$\varepsilon_{ij} = 2\nu \overline{\frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i}} \approx \frac{2}{3} \varepsilon \delta_{ij}. \quad (6.2.1)$$

In this case, the Reynolds stress equations become

$$\frac{\partial}{\partial t} (\overline{u_1 u_1}) = -2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} + 2 \overline{\frac{p}{\rho} \frac{\partial u_1}{\partial x_1}} - \frac{2}{3} \varepsilon, \quad (6.2.2a)$$

$$\frac{\partial}{\partial t} (\overline{u_2 u_2}) = 2 \overline{\frac{p}{\rho} \frac{\partial u_2}{\partial x_2}} - \frac{2}{3} \varepsilon, \quad (6.2.2b)$$

$$\frac{\partial}{\partial t} (\overline{u_3 u_3}) = 2 \overline{\frac{p}{\rho} \frac{\partial u_3}{\partial x_3}} - \frac{2}{3} \varepsilon, \quad (6.2.2c)$$

$$\frac{\partial}{\partial t} (\overline{u_1 u_2}) = -\overline{u_2 u_2} \frac{\partial U_1}{\partial x_2} + \overline{\frac{p}{\rho} \left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right)}, \quad (6.2.2d)$$

$$\frac{\partial}{\partial t} (\overline{u_1 u_3}) = -\overline{u_2 u_3} \frac{\partial U_1}{\partial x_2} + \overline{\frac{p}{\rho} \left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right)}, \quad (6.2.2e)$$

$$\frac{\partial (\overline{u_2 u_3})}{\partial t} = \overline{\frac{p}{\rho} \left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right)}. \quad (6.2.2f)$$

Summation of Eqs. 6.2.2a-6.2.2c gives

$$\frac{\partial k}{\partial t} = P - \varepsilon = -\overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - \varepsilon. \quad (6.2.3)$$

6.3 Modeled Reynolds Equations for Homogeneous Turbulence

The pressure-strain production term π_{ij} is modeled for isothermal flow by

$$\pi_{ij} = \overline{\frac{p}{\rho} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)} = \pi_{ij}^1 + \pi_{ij}^2 = -c_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) - c_2 \left(P_{ij} - \frac{2}{3} P \delta_{ij} \right), \quad (6.3.1)$$

with $c_1 = 2.8$ and $c_2 = 0.47$.

Using Eqs. 6.1.2 and 6.1.4, we obtain the following equations for the components of the tensor:

$$\pi_{11} = -c_1 \frac{\varepsilon}{k} \left(\overline{u_1 u_1} - \frac{2}{3} k \right) + \frac{4}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} = -c_1 \varepsilon a_{11} - c_2 \frac{2}{3} P_{11}, \quad (6.3.2a)$$

$$\pi_{22} = -c_1 \frac{\varepsilon}{k} \left(\overline{u_2 u_2} - \frac{2}{3} k \right) - \frac{2}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} = -c_1 \varepsilon a_{22} + c_2 \frac{P_{11}}{3}, \quad (6.3.2b)$$

$$\pi_{33} = -c_1 \frac{\varepsilon}{k} \left(\overline{u_3 u_3} - \frac{2}{3} k \right) - \frac{2}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} = -c_1 \varepsilon a_{33} + c_2 \frac{P_{11}}{3}, \quad (6.3.2c)$$

$$\pi_{12} = -c_1 \frac{\varepsilon}{k} \overline{u_1 u_2} + c_2 \overline{u_2 u_2} \frac{\partial U_1}{\partial x_2} = -c_1 \varepsilon a_{12} - c_2 P_{12}, \quad (6.3.2d)$$

$$\pi_{13} = -c_1 \frac{\varepsilon}{k} \overline{u_1 u_3} + c_2 \overline{u_2 u_3} \frac{\partial U_1}{\partial x_2} = -c_1 \varepsilon a_{13} - c_2 P_{13}, \quad (6.3.2e)$$

$$\pi_{23} = -c_1 \frac{\varepsilon}{k} \overline{u_2 u_3} = -c_1 \varepsilon a_{23}. \quad (6.3.2f)$$

Introducing Eqs. 6.3.2 into 6.1.3 we obtain the modeled Reynolds equations for homogeneous turbulence, i.e.,

$$\frac{\partial(\overline{u_1 u_1})}{\partial t} = -2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - c_1 \frac{\varepsilon}{k} \left(\overline{u_1 u_1} - \frac{2}{3} k \right) + \frac{4}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - 2 \nu \overline{\frac{\partial u_1}{\partial x_\ell} \frac{\partial u_1}{\partial x_\ell}}, \quad (6.3.3a)$$

$$\frac{\partial(\overline{u_2 u_2})}{\partial t} = -c_1 \frac{\varepsilon}{k} \left(\overline{u_2 u_2} - \frac{2}{3} k \right) - \frac{2}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - 2 \nu \overline{\frac{\partial u_2}{\partial x_\ell} \frac{\partial u_2}{\partial x_\ell}}, \quad (6.3.3b)$$

$$\frac{\partial(\overline{u_3 u_3})}{\partial t} = -c_1 \frac{\varepsilon}{k} \left(\overline{u_3 u_3} - \frac{2}{3} k \right) - \frac{2}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - 2 \nu \overline{\frac{\partial u_3}{\partial x_\ell} \frac{\partial u_3}{\partial x_\ell}}, \quad (6.3.3c)$$

$$\frac{\partial(\overline{u_1 u_2})}{\partial t} = -\overline{u_2 u_2} \frac{\partial U_1}{\partial x_2} - c_1 \frac{\varepsilon}{k} \overline{u_1 u_2} + c_2 \overline{u_2 u_2} \frac{\partial U_1}{\partial x_2} - 2 \nu \overline{\frac{\partial u_1}{\partial x_\ell} \frac{\partial u_2}{\partial x_\ell}}, \quad (6.3.3d)$$

$$\frac{\partial(\overline{u_1 u_3})}{\partial t} = -\overline{u_2 u_3} \frac{\partial U_1}{\partial x_2} - c_1 \frac{\varepsilon}{k} \overline{u_1 u_3} + c_2 \overline{u_2 u_3} \frac{\partial U_1}{\partial x_2} - 2 \nu \overline{\frac{\partial u_1}{\partial x_\ell} \frac{\partial u_3}{\partial x_\ell}}, \quad (6.3.3e)$$

$$\frac{\partial(\overline{u_2 u_3})}{\partial t} = -c_1 \frac{\varepsilon}{k} \overline{u_2 u_3} - 2v \frac{\partial \overline{u_2}}{\partial x_\ell} \frac{\partial \overline{u_3}}{\partial x_\ell}. \quad (6.3.3f)$$

If we use Eq. 6.2.1, the modeled Reynolds equations for homogeneous isotropic turbulence become

$$\frac{\partial(\overline{u_1 u_1})}{\partial t} = -2\overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - c_1 \frac{\varepsilon}{k} \left(\overline{u_1 u_1} - \frac{2}{3} k \right) + \frac{4}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - \frac{2}{3} \varepsilon, \quad (6.3.4a)$$

$$\frac{\partial(\overline{u_2 u_2})}{\partial t} = -c_1 \frac{\varepsilon}{k} \left(\overline{u_2 u_2} - \frac{2}{3} k \right) - \frac{2}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - \frac{2}{3} \varepsilon, \quad (6.3.4b)$$

$$\frac{\partial(\overline{u_3 u_3})}{\partial t} = -c_1 \frac{\varepsilon}{k} \left(\overline{u_3 u_3} - \frac{2}{3} k \right) - \frac{2}{3} c_2 \overline{u_1 u_2} \frac{\partial U_1}{\partial x_2} - \frac{2}{3} \varepsilon, \quad (6.3.4c)$$

$$\frac{\partial(\overline{u_1 u_2})}{\partial t} = -\overline{u_2 u_2} \frac{\partial U_1}{\partial x_2} - c_1 \frac{\varepsilon}{k} \overline{u_1 u_2} + c_2 \overline{u_2 u_2} \frac{\partial U_1}{\partial x_2}, \quad (6.3.4d)$$

$$\frac{\partial(\overline{u_1 u_3})}{\partial t} = -\overline{u_2 u_3} \frac{\partial U_1}{\partial x_2} - c_1 \frac{\varepsilon}{k} \overline{u_1 u_3} + c_2 \overline{u_2 u_3} \frac{\partial U_1}{\partial x_2}, \quad (6.3.4e)$$

$$\frac{\partial(\overline{u_2 u_3})}{\partial t} = -c_1 \frac{\varepsilon}{k} \overline{u_2 u_3}. \quad (6.3.4f)$$

Under the assumption of homogeneous turbulence, Eqs. 6.1.1 and 6.1.2, the equation for the dissipation of turbulent kinetic energy becomes

$$\frac{\partial \varepsilon}{\partial t} = c_{1\varepsilon} \frac{\varepsilon}{k} (-\overline{u_1 u_2}) \frac{\partial U_1}{\partial x_2} - c_{2\varepsilon} \frac{\varepsilon^2}{k}. \quad (6.3.5)$$

6.4 Integration of Modeled Reynolds Equations with Runge-Kutta Algorithm

In homogeneous turbulence, all of the averages are not spatial-dependent, but depend at most on time. Therefore, the partial derivatives in the above equations can be replaced by ordinary derivatives and the partial differential equations become ordinary differential equations of the first order. Equations 6.3.4 and 6.3.5 can be written in the compact form

$$\frac{d(\overline{u_1 u_1})}{dt} = \left(1 - \frac{2}{3} c_2 \right) P_{11} - c_1 \varepsilon a_{11} - \frac{2}{3} \varepsilon, \quad (6.4.1a)$$

$$\frac{d(\overline{u_2 u_2})}{dt} = \frac{c_2}{3} P_{11} - c_1 \varepsilon a_{22} - \frac{2}{3} \varepsilon, \quad (6.4.1b)$$

$$\frac{d(\overline{u_3 u_3})}{dt} = \frac{c_2}{3} P_{11} - c_1 \varepsilon a_{33} - \frac{2}{3} \varepsilon, \quad (6.4.1c)$$

$$\frac{d(\overline{u_1 u_2})}{dt} = (1 - c_2) P_{12} - c_1 \varepsilon a_{12}, \quad (6.4.1d)$$

$$\frac{d(\overline{u_1 u_3})}{dt} = (1 - c_2) P_{13} - c_1 \varepsilon a_{13}, \quad (6.4.1e)$$

$$\frac{d(\overline{u_2 u_3})}{dt} = -c_1 \varepsilon a_{23}, \quad (6.4.1f)$$

$$\frac{d\varepsilon}{dt} = c_{1\varepsilon} \frac{\varepsilon}{k} \frac{P_{11}}{2} - c_{2\varepsilon} \frac{\varepsilon^2}{k}. \quad (6.4.1g)$$

These equations are not linear because the values of a_{ij} are functions of the dependent variables. These equations have been numerically integrated with a Runge-Kutta scheme of order four with an adaptive time step.¹⁹

6.5 Numerical Results

The experiments reported in Ref. 18 were performed with a center velocity in the wind tunnel $U_c = 12.4$ m/s and a velocity gradient $\partial U_1 / \partial x_2 \approx 13$ s⁻¹. Measurements were taken in the region defined by $8.5H \leq x_1 \leq 10.5H$. 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 $x_1/H = 10$, which were reported in Ref. 18. A comparison of computed and experimental results is given in Table IV. 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, because of 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.

Another comparison between experimental and theoretical results can be made in terms of the diagonal components of the tensor a_{ij} , which represents the anisotropy of turbulence. This comparison is given in Table V. In Ref. 20, the Reynolds equations for homogeneous isotropic turbulence have been modeled in two ways, referred to in the table as Model 1 and Model 2.

Table IV. Experimental and computed turbulence values
in homogeneous shear flow

Turbulence Value	Experiment, Ref. 18	Calculations	
		Runge-Kutta	COMMIX-RSM
k	0.053	0.030	0.033
$\sqrt{k}/U_c$	0.0185	0.0139	0.0147
$\sqrt{\overline{u_1 u_1}}/U_c$	0.0178	0.0140	0.0143
$\sqrt{\overline{u_2 u_2}}/U_c$	0.0132	0.0097	0.0106
$\sqrt{\overline{u_3 u_3}}/U_c$	0.0141	0.0097	0.0106
$\sqrt{\overline{u_1 u_2}}/U_c$	0.0104	0.0101	0.0100
$P = \frac{P_k}{\rho} = -\overline{u_1 u_2} \frac{\partial U_1}{\partial x_2}$	0.218	0.203	0.201

Table V. Experimental and computed values of diagonal components of a_{ij} tensor

a_{ij} Component	Theoretical Models ²⁰		Experiment Ref. 18	Calculations	
	Model 1	Model 2		Runge-Kutta	COMMIX-RSM
$a_{11} = \frac{1}{k} \left(\overline{u_1 u_1} - \frac{2}{3} k \right)$	0.30	0.35	0.25	0.35	0.29
$a_{22} = \frac{1}{k} \left(\overline{u_2 u_2} - \frac{2}{3} k \right)$	-0.18	-0.175	-0.16	-0.175	-0.145
$a_{33} = \frac{1}{k} \left(\overline{u_3 u_3} - \frac{2}{3} k \right)$	-0.12	-0.175	-0.09	-0.175	-0.145

The only component of the turbulent kinematic viscosity term that can be defined under the conditions of Eq. 6.1.1, i.e., of homogeneous turbulence, is

$$v_{t12} = \frac{-\overline{u_1 u_2}}{\partial U_1 / \partial x_2}. \quad (6.5.1)$$

The computed value was $v_{t12} = -(-0.0155)/13 = 1.13 \times 10^{-3} \text{ m}^2/\text{s}$, which compares with the value $v_{t12} = 1.32 \times 10^{-3} \text{ m}^2/\text{s}$ reported in Ref. 18. Using $v_\ell = 1.45 \times 10^{-5} \text{ m}^2/\text{s}$ as in

Ref. 18, we obtain for the turbulent Reynolds number $Re_t = v_t / \nu_\ell = 82$, which compares well with $Re_t = 91$ of Ref. 18.

Further verification of the RSM has been made in cases of stable and unstable stratified shear flow between horizontal parallel plates and in cases of steady-state and transient, so-called thermal cavity, problems. Results of these verifications are documented in Ref. 21.

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