1987

Three-Dimensional Turbulent Flowfield in a Turbine Stirred Tank.

Sheng-yang Ju

Louisiana State University and Agricultural & Mechanical College

Follow this and additional works at: https://digitalcommons.lsu.edu/gradschool_disstheses

Recommended Citation
https://digitalcommons.lsu.edu/gradschool_disstheses/4403

This Dissertation is brought to you for free and open access by the Graduate School at LSU Digital Commons. It has been accepted for inclusion in LSU Historical Dissertations and Theses by an authorized administrator of LSU Digital Commons. For more information, please contact gradetd@lsu.edu.
INFORMATION TO USERS

While the most advanced technology has been used to photograph and reproduce this manuscript, the quality of the reproduction is heavily dependent upon the quality of the material submitted. For example:

- Manuscript pages may have indistinct print. In such cases, the best available copy has been filmed.

- Manuscripts may not always be complete. In such cases, a note will indicate that it is not possible to obtain missing pages.

- Copyrighted material may have been removed from the manuscript. In such cases, a note will indicate the deletion.

Oversize materials (e.g., maps, drawings, and charts) are photographed by sectioning the original, beginning at the upper left-hand corner and continuing from left to right in equal sections with small overlaps. Each oversize page is also filmed as one exposure and is available, for an additional charge, as a standard 35mm slide or as a 17”x 23” black and white photographic print.

Most photographs reproduce acceptably on positive microfilm or microfiche but lack the clarity on xerographic copies made from the microfilm. For an additional charge, 35mm slides of 6”x 9” black and white photographic prints are available for any photographs or illustrations that cannot be reproduced satisfactorily by xerography.
Three-dimensional turbulent flowfield in a turbine stirred tank

Ju, Sheng-Yang, Ph.D.
The Louisiana State University and Agricultural and Mechanical Col., 1987
PLEASE NOTE:

In all cases this material has been filmed in the best possible way from the available copy. Problems encountered with this document have been identified here with a check mark √.

1. Glossy photographs or pages ______
2. Colored illustrations, paper or print ______
3. Photographs with dark background ______
4. Illustrations are poor copy ______
5. Pages with black marks, not original copy ______
6. Print shows through as there is text on both sides of page ______
7. Indistinct, broken or small print on several pages √
8. Print exceeds margin requirements ______
9. Tightly bound copy with print lost in spine ______
10. Computer printout pages with indistinct print ______
11. Page(s) ________ lacking when material received, and not available from school or author.
12. Page(s) ________ seem to be missing in numbering only as text follows.
13. Two pages numbered ______. Text follows.
14. Curling and wrinkled pages ______
15. Dissertation contains pages with print at a slant, filmed as received ______
16. Other_________________________________________________________________

_________________________________________________________________

University
Microfilms
International
THREE-DIMENSIONAL TURBULENT FLOWFIELD
IN A TURBINE STIRRED TANK

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Chemical Engineering

by

Sheng-Yang Ju
B.S., National Taiwan University, 1980
M.S., Louisiana State University, 1984
August 1987
Acknowledgments

This research was carried out under the direction of Professor Ralph W. Pike. His time and support are sincerely appreciated. The examining committee members, Professors Martin A. Hjortso, Arthur M. Sterling, David M. Wetzel, Sumanta Acharya, and Gisele R. Rieder are thanked for their efforts in reviewing and evaluating this research. The assistance of Mr. Robert L. Schorr to prepare some figures in the second and third chapters is also appreciated.

The financial aid for this research by the Louisiana Mining and Mineral Resources Research Institute is gratefully acknowledged. Also, the Department of Chemical Engineering at LSU is recognized for its assistance and support.

Finally, the author would like to extend his deepest appreciations to his family.
# Table of Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acknowledgements</td>
<td>ii</td>
</tr>
<tr>
<td>List of Tables</td>
<td>vii</td>
</tr>
<tr>
<td>List of Figures</td>
<td>ix</td>
</tr>
<tr>
<td>Abstract</td>
<td>xiv</td>
</tr>
<tr>
<td>Chapter I - Introduction and Background</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Introduction</td>
<td>1</td>
</tr>
<tr>
<td>1.2 General Background for an Agitated Vessel</td>
<td>7</td>
</tr>
<tr>
<td>1.2.1 Characteristics of Agitated Vessels</td>
<td>7</td>
</tr>
<tr>
<td>1.2.2 Fluid Dynamics of Mixing</td>
<td>21</td>
</tr>
<tr>
<td>1.3 Summary and Objectives</td>
<td>23</td>
</tr>
<tr>
<td>1.4 References</td>
<td>26</td>
</tr>
<tr>
<td>Chapter II - Literature Review and Assessment</td>
<td>27</td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>27</td>
</tr>
<tr>
<td>2.2 Theoretical Studies</td>
<td>28</td>
</tr>
<tr>
<td>2.2.1 Numerical Solutions</td>
<td>28</td>
</tr>
<tr>
<td>2.2.2 Analytical Tank Region Simulation</td>
<td>38</td>
</tr>
<tr>
<td>2.2.3 Tangential Jet Model and Trailing Vortex Model</td>
<td>44</td>
</tr>
<tr>
<td>2.3 Experimental Studies</td>
<td>51</td>
</tr>
<tr>
<td>2.4 Summary</td>
<td>64</td>
</tr>
<tr>
<td>2.5 References</td>
<td>67</td>
</tr>
<tr>
<td>Section</td>
<td>Page</td>
</tr>
<tr>
<td>------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>70</td>
</tr>
<tr>
<td>3.2 Conservation Equations for Turbulent Flows</td>
<td>71</td>
</tr>
<tr>
<td>3.3 Mathematical Models of Turbulence</td>
<td>74</td>
</tr>
<tr>
<td>3.3.1 Isotropic Model</td>
<td>76</td>
</tr>
<tr>
<td>3.3.2 Nonisotropic Model</td>
<td>84</td>
</tr>
<tr>
<td>3.4 General Form of the Governing Equations</td>
<td>87</td>
</tr>
<tr>
<td>3.5 Boundary Conditions for the Transport Equations</td>
<td>88</td>
</tr>
<tr>
<td>3.6 Two-Dimensional Finite Domain Formulation</td>
<td>92</td>
</tr>
<tr>
<td>3.6.1 General Derivation</td>
<td>93</td>
</tr>
<tr>
<td>3.6.2 The Pressure Equation</td>
<td>106</td>
</tr>
<tr>
<td>3.6.3 Corrections of the Velocity Field</td>
<td>108</td>
</tr>
<tr>
<td>3.7 Extensions for a Three-Dimensional Flow Field</td>
<td>110</td>
</tr>
<tr>
<td>3.7.1 Conservation Equations in the Isotropic Model</td>
<td>110</td>
</tr>
<tr>
<td>3.7.2 Conservation Equations in the Nonisotropic Model</td>
<td>113</td>
</tr>
<tr>
<td>3.7.3 Boundary Conditions for Three-Dimensional Equations</td>
<td>117</td>
</tr>
<tr>
<td>3.7.4 Three-Dimensional Discretization Equations</td>
<td>117</td>
</tr>
<tr>
<td>3.8 Calculation Method</td>
<td>127</td>
</tr>
<tr>
<td>3.8.1 TDMA with Sweep Method</td>
<td>128</td>
</tr>
<tr>
<td>3.8.2 SIMPLE Algorithm</td>
<td>130</td>
</tr>
<tr>
<td>3.8.3 SIMPLER Algorithm</td>
<td>131</td>
</tr>
<tr>
<td>3.9 Boundary Conditions in Numerical Representations</td>
<td>133</td>
</tr>
<tr>
<td>3.10 Summary</td>
<td>138</td>
</tr>
<tr>
<td>3.11 References</td>
<td>140</td>
</tr>
</tbody>
</table>
Chapter IV - Results and Discussion

4.1 Introduction

4.2 Three-Dimensional Simulation

4.2.1 Solution from Nonisotropic Model

4.2.1.1 Velocity Field Description

4.2.1.2 Turbulence Field Description

4.2.2 Validation of Nonisotropic Model

4.2.2.1 Velocity Field Validation

4.2.2.2 Turbulence Field Validation

4.2.3 Comparison of Two Three-Dimensional Simulations

4.3 Two-Dimensional Simulation

4.3.1 Consideration of Drag Effects

4.3.2 Comparison of Four Two-Dimensional Simulations

4.4 Comparison of Previous Studies

4.4.1 Three-Dimensional Simulations

4.4.2 Two-Dimensional Simulations

4.5 Convergence and Accuracy

4.6 Algorithm Comparison

4.7 Summary

4.8 References

Chapter V - Conclusions and Recommendations

5.1 Conclusions

5.2 Recommendations
Nomenclature................................................. 228

Appendix A: Material Balance over the Blade-Swept Region..... 234
Appendix B: Figures for Tank Systems 2 and 3..................... 238
Appendix C: Program Listing.................................. 255
Appendix D: A Sample Output.................................. 327

VITA............................................................. 354
List of Tables

Table Page

I-1. Geometrical Relationships for the Standard Tank Configuration with a Turbine Impeller from Holland... 20
II-1. Standard versus Actual Tank Configuration Used by Mulvahill........................................ 52
III-1. Two-Dimensional Axisymmetric Governing Equations with the Isotropic Model...................... 89
III-2. Two-Dimensional Axisymmetric Governing Equations with the Nonisotropic Model.................... 90
III-3. Three-Dimensional Conservation Equations with the Isotropic Model.................................... 114
III-4. Three-Dimensional Conservation Equations with the Nonisotropic Model............................... 118
IV-1. Three Stirred Tank Systems.................................................. 144
IV-2. CPU Time in Minutes on FPS-264 for Two Three-Dimensional Simulations............................. 182
IV-3. Differences of Four Versions of Two-Dimensional k-ε Turbulence Model................................. 191
IV-4. CPU Time in Minutes on IBM 3084 for Four Two-Dimensional Simulations............................ 202
IV-5. Comparison of the Three-Dimensional Simulations for the Turbulent Flow in Agitated Vessels for Middleton, et al. and This Research................................. 204
IV-6. Comparison of the Two-Dimensional Simulations for the Turbulent Flow in Agitated Vessels for Platzer, Placek, et al., Harvey and Greaves, and This Research.... 207
IV-7. Relaxation Factors in Four Two-Dimensional Simulations of the Turbulent Flow in Three Stirred Tank Systems.... 212
IV-8. Relaxation Factors in Two Three-Dimensional Simulations of the Turbulent Flow in Three Stirred Tank Systems.... 212
IV-9. Nondimensional Velocity Components at \( r' = 3.46 \) and
z'=3.0 in Tank System 1 with Various Grids .......... 216

IV-10. CPU Time for the SIMPLE and SIMPLER Algorithms .......... 220

A-1. The Computed Values of Proportional Constant $\alpha$
     from the Two-Dimensional Simulations ................. 237
List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I-1. The flow pattern in a baffled mixing tank with a radial flow turbine from Holland</td>
<td>2</td>
</tr>
<tr>
<td>I-2. Power curve for a flat blade turbine from Ludwig</td>
<td>3</td>
</tr>
<tr>
<td>I-3. Seven basic impellers commonly used in chemical process industries plants from Oldshue</td>
<td>8</td>
</tr>
<tr>
<td>I-4. General selection chart for mixing from Ludwig</td>
<td>11</td>
</tr>
<tr>
<td>I-5. Vortex formation and circulation patterns in a stirred tank without baffles from Oldshue</td>
<td>14</td>
</tr>
<tr>
<td>I-6. Standard tank configuration from Holland</td>
<td>19</td>
</tr>
<tr>
<td>I-7. Tangential jet from DeSouza</td>
<td>22</td>
</tr>
<tr>
<td>I-8. Shear rate obtained from the velocity profile from Oldshue</td>
<td>24</td>
</tr>
<tr>
<td>II-1. Velocity profiles in the r-θ and r-z plane from Middleton, et al</td>
<td>30</td>
</tr>
<tr>
<td>II-2. Calculated and measured angular velocity profiles along r-direction in the impeller plane from Harveys and Greaves</td>
<td>32</td>
</tr>
<tr>
<td>II-3. Comparison of resultant velocity at the tank wall for N = 400 min⁻¹ and D₁ = D/y/3 from Placek, et al</td>
<td>36</td>
</tr>
<tr>
<td>II-4. Comparison of resultant velocity at the tank wall for N = 840 min⁻¹ and D₁ = D/y/4 from Placek, et al</td>
<td>37</td>
</tr>
<tr>
<td>II-5. Typical computer drawn solution of flowfiled with six regions from DeSouza and Pike</td>
<td>39</td>
</tr>
<tr>
<td>II-6. Comparison of velocity profiles in the impeller stream by DeSouza</td>
<td>41</td>
</tr>
<tr>
<td>II-7. Distribution of seven regions in stirred tanks</td>
<td>43</td>
</tr>
<tr>
<td>II-8. Distribution of eight regions in stirred tanks</td>
<td>45</td>
</tr>
<tr>
<td>II-9. Schematic 3-D view of the trailing vortex pair behind ix</td>
<td></td>
</tr>
</tbody>
</table>
each impeller blade (Top), and 2-D view of the flow field in the impeller region. S, stagnation point after Van't Riet and Smith

II-10. Axial velocity components on the 45° plane in the tank with 3" turbine at 250 rpm from Mulvahill

II-11. Angular velocity components along the θ-direction in three tank systems from Mulvahill

II-12. Normalized turbulence energy dissipation rates in the impeller stream from Patterson and Wu

III-1. Boundary conditions for flow in an agitated vessel

III-2. Locations of the grid points and control faces in a finite domain scheme

III-3 Spacings corresponding to the finite domain scheme in Figure III-2

III-4. Finite domain for the velocity in the z-direction

III-5. Finite domain for the velocity in the r-direction

III-6. Three-dimensional finite domain for a main grid point

III-7. Finite domain in the r-θ plane

III-8. Calculation domain in the r-θ plane

IV-1. The dimensionless velocity vectors on the 45° r-z plane in Tank System 1

IV-2. The dimensionless velocity vectors on the r-θ plane at the location of z'=2.5 in Tank System 1

IV-3. Turbulence kinetic energy on the r-θ plane at z'=0, the impeller plane, in Tank System 1

IV-4. Contours of turbulence kinetic energy on the 45° plane in Tank System 1

IV-5. Block diagrams of turbulence energy on the 45° plane in Tank System 1

IV-6. Energy dissipation rate of the impeller stream on the r-θ plane in Tank System 1

IV-7. Contours of energy dissipation rates on the
45° plane in Tank System 1 ............................................. 157

IV-8. Block diagrams of dissipation rates on the 45° plane in Tank System 1 ............................................. 158

IV-9. Radial velocity profiles along the θ-direction ............ 160

IV-10. Tangential velocity profiles along the θ-direction ....... 161

IV-11. Axial velocity profiles along the θ-direction ............. 162

IV-12. Radial velocity profiles along the r-direction on the 45° plane ............................................. 163

IV-13. Tangential velocity profiles along the r-direction on the 45° plane ............................................. 164

IV-14. Axial velocity profiles along the r-direction on the 45° plane ............................................. 165

IV-15. Axial profiles of turbulence kinetic energy in different radial positions of impeller streams on 45° plane .... 169

IV-16. Axial profiles of turbulence energy dissipation rates in different radial positions of impeller streams on 45° plane ............................................. 171

IV-17. Axial profiles of turbulence energy dissipation rates in Patterson and Wu's study and this work ............... 173

IV-18. Radial velocity profiles along the θ-direction obtained with two three-dimensional models .................. 174

IV-19. Tangential velocity profiles along the θ-direction obtained with two three-dimensional models ............. 176

IV-20. Axial velocity profiles along the θ-direction obtained with two three-dimensional models ................. 177

IV-21. Radial velocity profiles along the r-direction on the 45° plane obtained with two three-dimensional models ............................................. 178

IV-22. Tangential velocity profiles along the r-direction on the 45° plane obtained with two three-dimensional models ............................................. 179

IV-23. Axial velocity profiles along the r-direction on the 45° plane obtained with two three-dimensional models ............................................. 180
IV-24. The drag effects on velocity in the bulk region of Tank System 1. The number on the left in parenthesis is $C_{D_{\text{Drj}}}$, and the one on the right is $C_{D_{\text{Drb}}}$. 185

IV-25. The drag effects on velocity in the jet zone of Tank System 1. The number on the left in parenthesis is $C_{D_{\text{Drj}}}$, and the one on the right is $C_{D_{\text{Drb}}}$. 186

IV-26. The tangential velocity component in the jet zone for three tank systems with five pairs of drag coefficients. 188

IV-27. The tangential velocity in the bulk region of three tank systems with five pairs of drag coefficients. 189

IV-28. Radial velocity at three different axial positions in the discharge stream of three tank systems. 192

IV-29. Radial velocity at three different axial positions in the bulk regions of three tank systems. 194

IV-30. Tangential velocity at three different axial positions in the discharge stream of three tank systems. 195

IV-31. Tangential velocity at three different axial positions in the bulk regions of three tank systems. 197

IV-32. Axial velocity at three different axial positions in the discharge stream of three tank systems. 198

IV-33. Axial velocity at three different axial positions in the bulk regions of three tank systems. 200

IV-34. Accuracy checked by comparing the computed velocity profiles corresponding to four different meshes. 215

IV-35. Nondimensional velocity profiles computed with the SIMPLE and SIMPLER algorithm in the two-dimensional simulation of the turbulent flow in Tank System 1. 218

IV-36. Profiles for $k^\prime$ and $\varepsilon^\prime$ computed with the SIMPLE and SIMPLER algorithm in the two-dimensional simulation of the turbulent flow in Tank System 2. 219

B-1. Turbulence kinetic energy of the impeller stream on the r-0 plane in Tank System 2. 239

B-2. Turbulence kinetic energy of the impeller stream on the r-0 plane in Tank System 3. 240
B-3. Contours of turbulence kinetic energy on the 45° plane in Tank System 2................................. 241

B-4. Block diagrams of turbulence kinetic energy on the 45° plane in Tank System 2................................. 242

B-5. Contours of turbulence kinetic energy on the 45° plane in Tank System 3................................. 243

B-6. Block diagrams of turbulence kinetic energy on the 45° plane in Tank System 3................................. 244

B-7. Energy dissipation rate of the impeller stream on the r-0 plane in Tank System 2................................. 245

B-8. Energy dissipation rate of the impeller stream on the r-0 plane in Tank System 3................................. 246

B-9. Contours of energy dissipation rates on the 45° plane in Tank System 2................................. 247

B-10. Block diagrams of dissipation rates on the 45° plane in Tank System 2................................. 248

B-11. Contours of energy dissipation rates on the 45° plane in Tank System 3................................. 249

B-12. Block diagrams of dissipation rates on the 45° plane in Tank System 3................................. 250

B-13. The drag effects on velocity in the bulk region of Tank System 2. The number on the left in parenthesis is $C_{D_{rj}}$, and the one on the right is $C_{D_{rb}}$................................. 251

B-14. The drag effects on velocity in the jet zone of Tank System 2. The number on the left in parenthesis is $C_{D_{rj}}$, and the one on the right is $C_{D_{rb}}$................................. 252

B-15. The drag effects on velocity in the bulk region of Tank System 3. The number on the left in parenthesis is $C_{D_{rj}}$, and the one on the right is $C_{D_{rb}}$................................. 253

B-16. The drag effects on velocity in the jet zone of Tank System 3. The number on the left in parenthesis is $C_{D_{rj}}$, and the one on the right is $C_{D_{rb}}$................................. 254
Abstract

Solutions of conservation equations for the three-dimensional turbulent flowfield in agitated vessels were developed. Results showed that the Navier-Stokes equations with the nonisotropic k-ε turbulence model described the three-dimensional velocity profiles and turbulence kinetic energy and its dissipation rate for the flowfield. The nonisotropic model considered the rotational effect on turbulence with a turbulent-Richardson-number term and accounted for the important baffling effects through the nonisotropy of the viscosity. The solutions were validated with the experimental data for velocities by Mulvahill and for turbulence parameters by Patterson and Wu. An isotropic k-ε turbulence model for rotational flow was also used. This modified isotropic k-ε model proved to be inaccurate to describe the turbulent flow in turbine stirred tanks because it did not consider the baffling effects. We also compared this work with the similar studies by other investigators. These comparisons showed that the finite domain method and the nonisotropic k-ε model were the appropriate ones to be used in studies of the three-dimensional turbulent flow in agitated vessels.

The turbulent flowfield simulation used the Navier-Stokes equations and a turbulence model to form a closure system. We proposed and used two different k-ε models for this purpose. The three-dimensional transport equations were discretized with the finite domain method. The power law scheme was used to approximate the convective transport and diffusive flux. The discretization equations were solved with the SIMPLE algorithm.
In this solution procedure the Tri-Diagonal Matrix Algorithm with sweep method was used to solve each of the discretization equations. A general purpose computer FORTRAN code was developed to obtain solutions of these three-dimensional equations with the FPS-264 scientific computer.
1.1 Introduction

Mixing is a very important operation in the chemical and petroleum refinery industries. It is widely utilized to perform a number of functions. These include continuous stirred chemical reactors, absorption and extraction columns, and suspension, dispersion and blending operators. Also, other industrial applications of fluid mixing include coagulation, flocculation, polymerization, nitration, alkylation, fermentation, food processing, pulp and paper processing, etc.

In this chapter, we will briefly state why and how theoretical research on the fluid dynamics in mixing tanks should be performed. We will also introduce some important features associated with the agitated vessels as the background for this research. Finally, the research approach and objectives will be discussed.

As shown in Figure I-1, a flat-blade turbine is used to generate the three-dimensional turbulent flowfield in the baffled mixing vessels. This fluid motion is created to eliminate the temperature and concentration gradients in the fluid, to suspend solid particles, to maintain emulsions, and to disperse a gas phase into a liquid phase.

The design of mixing tanks and stirred reactors is mainly based on empirical knowledge. An example is the power curve, shown in Figure I-2, which correlates the power number and Reynolds number. This correlation
Figure I-1. The flow pattern in a baffled mixing tank with a radial flow turbine from Holland(1).
Figure I-2. Power curve for a flat blade turbine from Ludwig(2).
permits scaling based on geometric similarity, but this approach has its difficulties as will be discussed subsequently. For further progress in the field, a solution to the transport equations is required to predict the velocity, temperature and concentration fields in stirred reactors. Currently, a stirred reactor or agitated vessel is either designed after an existing one; or it is designed from the experimental data taken from a pilot scale unit. It is time-consuming and expensive to obtain data for scale-up. In addition, there is a problem associated with maintaining geometric, kinematic and dynamic similarities in scale-up. For geometric similarity all relevant dimensions have common constant ratios, for kinematic similarity all velocities have common constant ratios, and for dynamic similarity all force ratios are the same.

It is not possible to scale-up a reactor or mixer by having kinematic and dynamic similarities because the fluid property would have to change. For example, when the impeller diameter is increased, the fluid viscosity would have to increase to maintain the same values of the Reynolds number. Therefore, experiments and experience require time, effort and money be invested on small-scale stirred reactors and mixing vessels in order to acquire satisfactory results for the design of an industrial reactor or mixer.

With the advent of supercomputers, it is now feasible to attempt solutions to governing equations which describe the fluid behavior in a stirred chemical reactor or mixing vessel. These solutions can be attained through a numerical solution of the conservation equations, frequently called computational fluid dynamics, CFD. The standard approach as described by Patterson(3) is to develop a numerical solution of the conservation equations for mass, momentum and energy which is validated by the experimental measurements from a pilot plant. Then the
numerical solution can be extrapolated to industrial scale with confidence since the analysis is based on the conservation laws. Therefore, it is possible to design the reactors or mixers based on first principles rather than empirical correlations.

Describing the fluid dynamics in the tank is the first and basic step in research on transport phenomena and chemical reactions in stirred reactors or mixers. A precise description of the fluid dynamics must be available to be used with the other transport equations. This must include a turbulence model for the turbulent flow. The turbulence model is required to describe the turbulent stress terms in the Navier-Stokes equations. These terms are the time-averaged products of the fluctuating components of the fluid velocity. They can be expressed in terms of an effective viscosity which appears in the classic energy-dissipation (k-ε) two-equation model. This turbulence model is listed below and these equations are conservation laws that have been used in numerous studies:

\[ \frac{\partial k}{\partial t} = \frac{\partial}{\partial x_j} \left( \frac{\mu_{\text{eff}}}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + \nu_T \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \frac{\partial V_i}{\partial x_j} - \rho \varepsilon \]  

(I-1)

\[ \frac{\partial \varepsilon}{\partial t} = \frac{\partial}{\partial x_j} \left( \frac{\mu_{\text{eff}} \varepsilon}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) + C_1 \frac{\varepsilon}{k} \nu_T \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) \frac{\partial V_i}{\partial x_j} - C_2 \rho \varepsilon^2 \]  

(I-2)

where the effective viscosity \( \mu_{\text{eff}} \) is the sum of the laminar viscosity, \( \mu \), and turbulent viscosity, \( \mu_T \). The turbulent viscosity is defined in terms of the turbulent kinetic energy \( k \) and its dissipation rate \( \varepsilon \) as given below.

\[ \nu_T = C_\mu \rho k^2 / \varepsilon \]  

(I-3)

To predict the turbulent velocity field, the time-averaged continuity and momentum equations, equations (I-4) and (I-5), are solved simultaneously.
with the turbulence model, i.e. equations (I-1) and (I-2) with the boundary and initial conditions for the flow.

\[
\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u_1}{\partial x_1} \quad (I-4)
\]

\[
\frac{\partial \rho u_1}{\partial t} = -\frac{\partial \rho}{\partial x_1} + \frac{\partial}{\partial x_j}(\nu_{eff} \frac{\partial u_1}{\partial x_j}) + \rho g_1 \quad (I-5)
\]

The derivation of the $k$-$\varepsilon$ model is described in Chapter III, and this model is obtained from manipulation with the momentum equations and other transport equations for the Reynolds stresses to form a closure system for turbulent flow. There is an approximation being made in the definition of the turbulent eddy viscosity, and no universal turbulence model exists. Consequently, it will be necessary to examine several turbulence models to be able to accurately describe the turbulent flow behavior in agitated vessels.

To date, no turbulence model has been satisfactory for the description of the turbulent flowfield in agitated vessels. However, some researchers have reported two- and three-dimensional solutions to the Navier-Stokes equations for studies in a dispersed phase system(4) and a simple competitive-consecutive reaction system(5).

Based upon the above discussion, we see that a numerical solution of the equations of motion is required with the aid of a turbulence model suitable for the flow in an agitated vessel. Because of the non-linearity and the coupling of these equations, an analytical solution is not feasible, and a numerical solution is required. A well-developed and tested numerical formulation and solution algorithm will be necessary in this work in order to obtain reliable and convergent results.

It is necessary to have velocity profiles measured in a stirred tank to verify the solutions of Navier-Stokes equations. A number of methods have
been tried to measure the three-dimensional velocities in agitated vessels. Some of these methods are laser doppler anemometry, hot wire anemometry, ion-specific probes, three-dimensional pitot tubes, photography of tracer particles, and fluorescence based concentration measurement. The most complete set of data was obtained by Mulvahill(6) who used a three-sensor hot wire anemometer to measure time-averaged or mean velocity profiles in a stirred vessel with the standard tank configuration, following developments of this method by others(7,8). His results are available for use to verify the velocity profiles obtained from the solution of the conservation equations in this research.

1.2 General Background for an Agitated Vessel

In this section a brief discussion of industrial mixing technology will be summarized to provide a perspective of the applications for this research. A mixing tank is composed of a power unit (motor), a driving unit (turbine or propeller) and a cylindrical vessel, and baffles are used to prevent vortex formation. In the next section, the characteristics of these baffles are described.

1.2.1 Characteristics of Agitated Vessels

This section will briefly describe the important features of an agitated vessel. These include impeller characteristics, power consumption, baffling effects, and tank configuration.

Impeller Characteristics: Figure I-3 shows the seven basic types of impellers commonly found in chemical process industries plants. Impellers are generally classified in two basic categories, according to their discharge flow. Some (R1-R3) are radial flow impellers because they
<table>
<thead>
<tr>
<th>Number</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>R-1</td>
<td>Flat blade</td>
<td>Vertical blades bolted to support disk</td>
</tr>
<tr>
<td></td>
<td>R-2</td>
<td>Bar turbine Six blades bolted/welded to top and bottom of support disk</td>
</tr>
<tr>
<td>R-3</td>
<td>Anchor</td>
<td>Two blades with or without cross arm</td>
</tr>
<tr>
<td>A-1</td>
<td>Propeller</td>
<td>Constant pitch, skewed-back blades</td>
</tr>
<tr>
<td>A-2</td>
<td>Axial flow</td>
<td>Constant angle at 45°</td>
</tr>
<tr>
<td>A-3</td>
<td>Axial flow</td>
<td>Variable blade angle, near constant pitch</td>
</tr>
<tr>
<td>A-4</td>
<td>Double spiral</td>
<td>Two helical flights, pitch = 100</td>
</tr>
</tbody>
</table>

**Figure I-3.** Seven basic impellers commonly used in chemical process industries plants from Oldshue(9).
discharge a fluid in the direction of the impeller radius. Others (A1-A4) are termed as axial flow impellers because the principal locus of flow occurs along the axis of the impellers. Axial flow impellers include three-blade marine propellers and pitched blade turbines, and radial flow impellers include flat and curved blade turbines, bar turbines, and two-blade curved paddles.

The impeller shown as R1 in Figure I-3 is generally known as the Rushton turbine. It is used when fairly high shear and turbulence levels are required. A bar turbine, R2 in Figure I-3, creates the highest shear rates among the seven type of impellers. The anchor impeller, R3, is a contoured two-blade device and is utilized for heat transfer and blending when the fluid viscosity is between 5,000 and 50,000 cP.

The marine-type propellers, A1 of Figure I-3, are normally employed to create axial flow. They are used either on side-entering mixers or are mounted with the shaft of the propellers at an angle to the centerline of a mixing reactor tank to reduce vortex formation. The four-blade forty five degree pitched turbine, A2, is principally used for flow-controlled operation. The next type, A3, performs like a marine impeller, but it weighs less and is less expensive than marine impellers. The last one, A4, is a double spiral impeller, and is designed for very viscous fluids and has two helical flights. The inner flight pumps downward while the outer one pumps upward.

Mixing effects and fluid flow phenomena in agitated vessels are not clearly understood, and decisions about the best flow pattern, or what type and what size of impellers are desirable, depends on the experience and the applications. These decisions involve several considerations, such as the impeller power consumption, the rate of circulation desired, the viscosity of the fluid, the degree of shear (or turbulence), etc. At
present, only a qualitative understanding is available to design agitated vessels for various applications. For example, with a constant power consumption, smaller impellers at faster speeds are employed if high shear rates are desired. For extremely high shear rates, narrow-blade impellers, such as saw-tooth impellers and bar turbines, are recommended for dispersions of either liquids or solids in liquids; and a relatively high power input is required. Conversely, if high circulation rates are required with lower shear rates, larger impellers at lower speeds are used. Processes such as liquid-liquid and gas-liquid mass transfer require a higher power per unit volume than all liquid systems, and the radial flow impeller is then used. Axial flow impellers, including pitched-blade turbines and propellers, are generally required in applications such as solids suspension, blending and heat transfer that require high pumping capacity. A general chart(2), shown in Figure I-4, can be used to aid in the selection of a suitable impeller for the mixing application. This chart allows one to select the type of impeller for a particular application if the criteria for mixing are known. To ensure this selection is best, experimental measurements on the flow in the tank of interest are necessary.

As previously mentioned, however, experiments are expensive and time-consuming. Consequently, solution to the equations of motion for the flow in agitated vessels is the only alternative.

**Power Consumption:** Power consumption is another important factor in the design of a stirred tank. The turbulent flow in an agitated vessel is produced with an impeller, which converts the electric energy in the motor to the kinetic energy of the fluid. The power supplied by a mixer is absorbed through the friction in viscous and turbulent shear forces and
<table>
<thead>
<tr>
<th>Service</th>
<th>Mixing Device</th>
<th>Range</th>
<th>Criteria</th>
<th>Torq Diameter to Impeller Dia. Ratio</th>
<th>Torq Height to Dameter Ratio</th>
<th>Impadders and Position</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blending</td>
<td>Turbine Propeller Paddle</td>
<td></td>
<td>1. Volume Circulation</td>
<td>3:1 to 6:1</td>
<td>Unlimited</td>
<td>Single or Multiple</td>
</tr>
<tr>
<td>Dispersion (Immiscible Systems)</td>
<td>Turbine Propeller Paddle</td>
<td></td>
<td>1. Drop Size Control 2. Re-Circulation</td>
<td>3:0:1 to 3:5:1</td>
<td>1:1 to 1:2</td>
<td>In Staged Mixers</td>
</tr>
<tr>
<td>Reactions in Solution (Miscible Systems)</td>
<td>Turbine Propeller Paddle</td>
<td></td>
<td>1. Intensity 2. Volume Circulation</td>
<td>2:5:1 to 3:5:1</td>
<td>1:1 to 3:1</td>
<td>Single or Multiple</td>
</tr>
<tr>
<td>Dissolution</td>
<td>Turbine Propeller Paddle</td>
<td></td>
<td>1. Shear 2. Volume Circulation</td>
<td>2:0:1 to 3:5:1</td>
<td>1:1 to 1:2</td>
<td>At/or Below Center Line of Liquid Charge</td>
</tr>
<tr>
<td>High Viscosity Applications</td>
<td>Turbine Propeller Paddle</td>
<td></td>
<td>1. Volume Circulation 2. Low Velocity</td>
<td>2:0:1 to 3:2:1</td>
<td>2:1 to 3:1</td>
<td>Single or Multiple</td>
</tr>
<tr>
<td>Crystallization or Precipitation</td>
<td>Turbine Propeller Paddle</td>
<td></td>
<td>1. Circulation 2. Low Velocity 3. Shear Control</td>
<td>2:0:1 to 3:2:1</td>
<td>2:1 to 1:1</td>
<td>Single, At/or Below Center Line of Liquid Charge</td>
</tr>
</tbody>
</table>

Figure I-4. General selection chart for mixing from Ludwig(2).
then dissipates as heat. The consumption of power is a function of the type, size and numbers of the impeller; the fluid viscosity and density; the location and mounting type of the impeller; the speed of rotation and flow circulation rate; and the tank's geometry, dimensions and internal attachments (such as baffles). These variables make power requirement estimation only approximate. The power required to drive different types of impellers, however, can be determined from correlations of experimental data for those systems and/or configurations, e.g. the power curve for the standard tank configuration shown in Figure 1-2.

Impeller power is usually expressed in terms of two dimensionless quantities, i.e. the power number $N_p$ and Reynolds number $N_{Re}$. These quantities are defined by:

$$N_p = \frac{P g_c}{\rho N^2 D_i^5} \quad (I-6)$$

$$N_{Re} = D_i^2 N_p/\mu \quad (I-7)$$

where $P$ is the power input to the impeller, $D_i$ is the impeller diameter, $N$ is the impeller speed, $\mu$ is the fluid viscosity, and $g_c$ is a conversion factor for British units.

For geometrically similar, baffled tanks, it has been shown(2) that the power number and Reynolds number can be correlated by the following equation:

$$N_p = K_1 (N_{Re})^x \quad (I-8)$$

$K_1$ and $x$ are two empirical constants which are determined from experimental data.

According to Holland(1), the onset of turbulence in agitated vessels is a gradual process, and turbulence starts at $N_{Re}=20$. However, the flow is
primarily in laminar region at $N_{Re} \leq 400$, and the following correlation can be used to compute the power number and the power required to drive the impeller.

$$N_p = K_2(N_{Re})^{-1} \quad (I-9)$$

There is no simple correlation for the turbulent flow in the range of Reynolds number between 400 and 10,000. When $N_{Re}$ is over 10,000, the power number is constant for a tank containing four equally spaced baffles. In this case the power number is given by:

$$N_p = K_3 \quad (I-10)$$

In the above equations $K_2$ and $K_3$ are constants for impellers(10). For example, they can be obtained from Figure I-2 for a six flat blade turbine.

For those tanks with a centrally located impeller but with no baffles, the fluid begins swirling and a vortex forms as shown in Figure I-5. To take this into account, equation (I-8) then needs to be modified by including the effect of gravity which is not important in baffled tanks. Correlation for this case is:

$$N_p = K_1(N_{Re})^x (N_{Fr})^y \quad (I-11)$$

where $x$ and $y$ are determined by experiments for different impellers, and $N_{Fr}$, the Froude number, is defined by

$$N_{Fr} = D_l N^2 / g \quad (I-12)$$

One of the most useful correlations for the design of unbaffled tanks, which are usually used for highly viscous fluids, is given by:
(a) Axial flow propeller

(b) Radial flow turbine

Figure 1-5. Vortex formation and circulation patterns in a stirred tank without baffles from Oldshue(9).
\[ N_p = K_3(N_{Fr})^{(a-\log N_{Re})/b} \]  

(1-13)

where values of \( a \) and \( b \) are given by Rushton, Costich and Everett(11).

In summary, power number versus Reynolds number correlations have been reported for various types of impellers in both baffled tanks and unbaffled tanks(2,10,11). \( K \) values can be obtained from the power curves such as Figure I-2 to compute power requirements for the different impellers.

**Baffling Effects:** In an unbaffled mixing tank, a top-entering, centrally-located impellers will cause the fluid to flow only tangentially in the tank as shown in Figure I-5. For most applications, however, this situation is not desirable because the mere rotation of the fluid induces low shear rates and accordingly ineffective mixing. Moreover, if a high impeller speed is applied, a vortex forms around the shaft of the impeller and causes air entrainment into the fluid.

Properly designed baffles eliminate vortex formation and convert the tangential flow into the axial and radial flow. They provide a flow pattern that carries the flow in the tank through the impeller zone. An overbaffling design will reduce the flow rate and confine the flow between baffles, and may lead to a poor mixing performance. Proper design of tank baffles is done by experiments and experience, and standard baffles are four vertical side-wall baffles projecting about 1/10 to 1/12 of the tank diameter into the tank. This design converts most of the tangential flow to axial and radial flow, and consequently gives significantly better mixing.

In summary, baffles are necessary for the following reasons. They convert the tangential flow from the impeller into flow with axial and
radial components. Also, they prevent vortexing, i.e. excess swirling action and air induction, ensure a stable and consistent power consumption, and give a consistent correlation of the power number and Reynolds number.

It should be pointed out that for those mixing tanks in which vortexing action are not serious or does not exist, baffles are not necessary. One example is the mixing tank with a top-entering, off-centrally located impeller. Side-entering mixers are another example. They will be discussed briefly in next subsection along with a review on the tank configuration.

**Tank Configuration and Impeller Location:** A vertical, cylindrical mixing tank filled with a fluid to the height equal to the tank diameter is often used as a base point for describing an effect of geometry. For some applications, such as solid suspension and blending, a better ratio of the liquid height to the tank diameter is about 0.6 to 0.7 for minimum power consumption(9). Also, other factors may be taken into account for a proper choice of tank shape and geometry.

A single impeller can usually operate at fluid coverages from a half to two diameters of the impeller. The placement of an impeller can seriously affect its performance. For a propeller in a properly baffled system, axial fluid flow is produced as mentioned before. If the propeller is placed close to the bottom of a tank, the flow becomes radial, and the propeller operates like a flat turbine. Also, if a high rotational speed is used, then a swirling action develops at the bottom. For a rule of thumb the impeller should be mounted at a point of 1/6 of liquid depth off the tank bottom(9).
The impeller mounting is also governed by the location where the fluid is withdrawn. In the tank equipped with a turbine, the preferred location for the draw-off of mixed fluids is at the side opposite the turbine impeller(9). In a tank equipped with a propeller, it is best to draw off the fluid from the tank directly below the agitator so that suspended solids and mixed liquids can be removed as uniformly as possible(9). A study of the flow pattern of the mixing system should be made to assure that the desired mixed fluids are not only obtained but also withdrawn.

Mixers can be classified according to how impellers are mounted. There are two categories: side-entering mixers and top-entering mixers(12). The impellers of side-entering mixers, usually propellers, are normally placed above a flat tank bottom with the shaft horizontal, and at a 7° to 10° horizontal angle with a vertical plane through the centerline of the tank. This equipment is used for those fluids having a viscosity of up to 500 cP(13). For fluids with a viscosity from 500 to 5,000 cP, the mixer is usually top-entering. Compared with the side-entering mixers at a given power, top-entering ones operate at lower speeds with larger impellers. Because the top-entering mixers create the highest fluid flow at constant power, they are employed more often than side-entering ones(12). Both radial and axial flow impellers are used for top-entering mixers.

To avoid the swirling action and vortex formation, baffles are always needed as mentioned before. In normal practice there is a space between the tank wall and the baffles equal to about 1/3 of the baffle width. For fluids with high viscosity, e.g. 5,000 cP, baffle width may be reduced and baffle location may be changed to halfway between the tank wall and the impeller(9). To reserve some space at the bottom of the tank is also desirable for preventing solids from depositing. Angular off-center placement for top-entering impellers without baffles can eliminate
vortexing and swirling phenomena, too. However, this type of impellers requires more power than central ones due to the higher torque applied on the impeller shaft(9) for the same level of mixing.

The Standard Tank Configuration: The vessel configuration shown in Figure I-6 is known as the standard tank configuration which was defined by Holland(1) as one that provides adequate mixing for most processing requirements found in industry. The geometrical relationships of the standard tank configuration are given in Table I-1. According to Holland's definition, the recommended impeller diameter is one-third of the tank diameter, and the clearance of the impeller above the tank bottom is given as one impeller diameter. The standard tank configurations for various types of impellers are also governed by the correlation for power consumption. This means that variations in the parameters of a given mixing system, such as the impeller speed or the impeller diameter, are kept in a range where the power number is constant. For instance, Rushton, et al.(11) found that $N_p$ did not change for the ratios of the impeller diameter to the tank diameter ranging from 0.14 to 0.50 for the Rushton turbines (the turbine impellers with six-blade disc). Also, it has been shown that the power number is not affected for the impeller clearance from the tank bottom to the impeller diameter ratios ranging from 0.35 to 2.50 for two-blade turbines(14), although the impeller clearance normally used is one impeller diameter. Thus, the standard tank configuration is not unique, and some flexibility is admissible.

In practice, wide deviations from the standard tank configuration have been used in industrial mixers(1). Some of these were necessary due to the need for feeding or withdrawing fluids during the mixing process. Nevertheless, this configuration is widely used, especially for research;
Figure I-6. Standard tank configuration from Holland(1).
Table I-1. Geometrical Relationships for the Standard Tank Configuration with a Turbine Impeller from Holland(1).

<table>
<thead>
<tr>
<th>(1) Agitator Type</th>
<th>Six Flat Blade Disc Turbine (Rushton Turbine)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Impeller Diameter</td>
<td>1/3 Tank Diameter</td>
</tr>
<tr>
<td>(3) Impeller Height from Tank Bottom</td>
<td>1 Impeller Diameter</td>
</tr>
<tr>
<td>(4) Impeller Blade Width</td>
<td>1/5 Impeller Diameter</td>
</tr>
<tr>
<td>(5) Impeller Blade Length</td>
<td>1/4 Impeller Diameter</td>
</tr>
<tr>
<td>(6) Length of Impeller Blade Mounted on Central Disc</td>
<td>1/8 Impeller Diameter</td>
</tr>
<tr>
<td>(7) Liquid Height</td>
<td>1 Tank Diameter</td>
</tr>
<tr>
<td>(8) Baffle Number</td>
<td>Four</td>
</tr>
<tr>
<td>(9) Baffle Width</td>
<td>1/10 Tank Diameter</td>
</tr>
</tbody>
</table>
and the results obtained from different researchers who used similar configuration are comparable.

For this work, the Rushton turbine is located midway between the fluid surface and the tank bottom. This is the configuration used by Mulvahill\cite{6} to measure the velocity profiles. The flow patterns in a mixing tank with this standard configuration were sketched in Figure I-1. The fluid is discharged from the turbine as a tangential jet, and the higher velocity fluid from the jet entrains the fluid around it. This flow divides at the tank wall, with one part flowing to the lower half of the tank which then loops around and up into the impeller zone. The other part flows upwards and then loops back down to the turbine. In addition, the fluid flows tangentially in the direction of rotation of the impeller.

1.2.2 Fluid Dynamics of Mixing:

We have discussed important characteristics of the baffled tank with an impeller in the previous subsection. Now we will briefly introduce the fluid flow phenomena of the mixing process. As mentioned before, the flow in an agitated vessel is created by a rotating impeller driven by a motor. The pumping capacity is defined as the volumetric flow rate of fluid which was radially or axially discharged from the impeller. The velocity distribution of the discharge flow from a radial flow impeller such as the flat blade turbine has been described by a turbulent tangential jet, which is illustrated in Figure I-7. The discharge area of a typical radial flow turbine with flat blades can be viewed as a cylindrical surface since the radial velocity component is dominant in the fluid flow discharge from this kind of impeller.
Figure I-7. Tangential jet from DeSouza(15)
Entrainment is an important element in mixing operations. It involves incorporation of low velocity fluid into the fluid stream or jet issuing from the mixing impeller source. Under proper conditions, the radial flow from a turbine serves as a circular cross-section jet to create mixing by turbulence as well as by entrainment.

Fluid elements intermix in a stirred tank by exchanging mass and momentum. Due to velocity differences layers of fluid intermingle with one another. In order to obtain velocity gradients, the impeller provides a high velocity flow field. A portion of the velocity profile for radial flow turbine is shown in Figure 1-8. It illustrates the velocity gradients obtained for the impeller. The velocity gradients are important in the design of mixers for chemical processes. These gradients are responsible for the reduction of particle sizes and the dispersion of gas bubbles or droplets(9).

1.3 Summary and Objectives

As discussed in the previous sections, the turbulent fluid dynamics of a mixing tank is very important. Patterson(16) pointed out that it is the key element for completely modeling chemical reactions and other processes in agitated vessels. Our research is an effort to make contributions in this area, and thus the characteristics and flow phenomena in agitated vessels have been introduced as background for our research.

In this research we will obtain a three-dimensional solution of the Navier-Stokes equations with an appropriate turbulence model to describe the fluid dynamics and turbulence phenomena in a stirred tank. A flexible and reliable numerical approach will be used to solve the partial
Figure I-8. Shear rate obtained from the velocity profile from Oldshue(9).
differential equations. We will develop a computer program, based on the numerical approach used, to compute the velocity profiles and turbulence parameters. The three-dimensional computer code will be designed so it can be applied to predict temperature and species concentration profiles for the further research in mixing. The validity of the solution for the velocity field and turbulence parameters will be verified by comparing the computed results with the experimental data. Also, an analysis of turbulence models will support the one used for the solution.
1.4 References


2.1 Introduction

In Chapter I, a brief introduction to mixing practice in mechanically agitated vessels has been presented. Also, the characteristics and fluid dynamics of agitated vessels were provided in some detail, and a summary and the objectives of this work were then stated in the final section. In this chapter, previous studies of the fluid flow phenomena in the baffled mixing tanks with a turbine impeller will be reviewed. An assessment will emphasize the theoretical and experimental studies which describe the fluid flow in agitated vessels with the standard tank configuration. This has been an active field of research for the past thirty years with numerous experimental and theoretical studies on various aspects of the turbulent fluid dynamics and its effect on the transport processes taking place in the vessel. First, the theoretical studies will be reviewed, and this will be followed by the experimental studies. This assessment will identify the state of knowledge in both these areas and be used as a basis for this research. Note that this review is for baffled tanks, since unbaffled vessels are only used for high viscosity fluids and research(1-4) has been essentially on the vortex shape and depth.
2.2 Theoretical Studies of the Turbulent Flow in Agitated Vessels

Four numerical and three analytical studies of the turbulent flow in agitated vessels with radial flow turbines have been reported in the literature. The flow in the impeller stream has been the active subject because of its importance, and two approaches have been developed which are the tangential jet and trailing vortex models. For flow in agitated vessels with an axial flow impeller, Fort(5) has published an indepth review of his and related research for this two-dimensional flow.

2.2.1 Numerical Solutions

As mentioned in Chapter I, turbulent flow can be described by solving the time-averaged continuity and momentum equations and a turbulence model. A numerical solution on a digital computer is required. In this section, the four previous numerical studies on the turbulent flow in agitated vessels will be reviewed. Among them, only one is three-dimensional. The other three are two-dimensional on the r-z plane based on the axisymmetry assumption.

Three-Dimensional Simulation by Middleton, et al.(5, Chapter I)*:

Middleton, et al.(5, Chapter I) have reported the only three-dimensional simulation of the turbulent flow in baffled stirred tanks using the numerical technique, known as finite domain method with SIMPLE algorithm, and the corresponding computer code developed at Imperial College in England. They solved the continuity and momentum equations along with the standard k-ε model, i.e., equation (I-1) to (I-5), for the turbulent

* (5, Chapter I) stands for the reference number of the cited literature in Chapter I.
flowfield first, and then they applied the computed flowfield results in a second program to describe the conversion of two competitive-consecutive chemical reactions in a stirred reactor. The boundary conditions at the impeller blades were obtained from the measurements by laser anemometry. They made a tabulated comparison of 16 experimental and computed final species concentrations and conversion fractions in 30 liter and 600 liter vessels, but there was no comparison with experimental data for the velocity profiles and turbulence parameters. The only results for the velocity profiles are shown in Figure II-1, and their plots clearly indicated how baffles affected the fluid motion. However, the important point is that they did not report any experiments or comparisons to establish the accuracy or validity of their solution for the fluid dynamics in the reactors. The validation of their results was based on the agreement of final concentrations in agitated vessels. They also showed the inapplicability of scale-up using power per volume, impeller tip speed or mixing time with their computed results.

Two-Dimensional Simulation by Harvey and Greaves(6):

Harvey and Greaves(6) developed a two-dimensional solution of the continuity equation and the momentum equations along with the standard k-ε turbulence model for the turbulent flow in an agitated vessel. They simplified the conservation equations by assuming axisymmetry, which neglects the three-dimensional character of the flow caused by the baffles, as shown in Figure II-1. To compensate for this assumption, they replaced the term $-(1/r)(\partial P/\partial \theta)$ in the angular momentum equation with what was called a pressure induced drag term, $-C_{Dr} \rho W^2/r$, to account for the baffling effects on the angular momentum field. $C_{Dr}$ was a model parameter determined by a best fit with experimental data. They simulated the
Figure II-1. Velocity profiles in the r-θ (Left) and r-z plane reported by Middleton, et al. (5, Chapter I)
mixing tank system of Gunkel and Weber(7) such that these experimental results for air agitated with a turbine could be used for comparison. Some of their theoretical results are compared with these data in Figure II-2 for profiles of the angular velocity along the r-direction in the impeller plane for a range of values for $C_D^r$. For this range of $C_D^r$, the difference between the theoretical results and experimental data is up to 100%. Comparisons of the theoretical and experimental angular velocities in other regions of the mixing tank are not reported. The differences between numerical and experimental profiles for the other two velocity components are comparable to that shown for the angular component. Also, Fort(8) claimed his eight-region analytical model(9) was more accurate than this model.

In summary, the turbulent flow model proposed by Harvey and Greaves(6) had the assumption of axisymmetry about the impeller shaft. However, the actual flow in a baffled mixing tank is three-dimensional, and neglecting the $\theta$-gradients leads to errors. Also, the angular momentum equation had to be modified by an empirical drag term to approximate the turbulent rotating flow in baffled tanks. In addition, there were incorrect boundary conditions used, and later they corrected the boundary conditions(10).

Two-Dimensional Simulation by Platzer(11):

Platzer(11) studied the turbulent flow of a stirred tank in which the impeller was not located in the center of the liquid height. He also assumed axisymmetry of the flowfield and eliminated all the $\theta$-gradients in the governing equations. To eliminate the difficulty caused by the pressure field, he utilized the stream function and vorticity transformations. He did not use a drag term in the angular momentum
Figure II-2. Calculated and measured angular velocity profiles along r-direction on the impeller plane from Harvey and Greaves(6).
equation to purposely reduce the tangential velocity to account for the baffling effects. The computed radial velocity profiles showed some deviation from velocity profiles of air measured with a hot wire anemometer in a turbine-agitated 0.0351m diameter vessel. Comparatively, other computed velocity profiles had more closely matched the data. A comparison for measured and computed turbulence kinetic energy has been made, also. However, the size and scale on these diagrams are such that it can be said that only qualitative agreement had been achieved. Consequently, it appeared that the two-dimensional simulation of the flow with the classic k-ε turbulence model could be improved to describe the turbulent flow in baffled stirred tanks. In addition, the use of stream function and vorticity transformations prohibits this analysis from being extended to three dimensions, since these transformations do not exist for three-dimensional flow.

Two-Dimensional Simulation by Placek, et al.(12):

Placek, et al.(12) reported that one previous numerical study by Placek(13), which used the standard k-ε turbulence model, could not accurately describe the turbulent flow in agitated vessels. Therefore, they proposed a modification by splitting the original k-equation to two equations: one for the large-scale convective vortices, \( k_p \), and the other for the transfer eddies, \( k_T \). The third scale of turbulence, i.e., dissipation eddies, was assumed negligible. The \( \varepsilon \)-equation they used was expressed in terms of \( k_p \) and \( k_T \). This two-scale three-equation turbulence model was composed of the following equations:

\[
\frac{Dk_p}{Dt} = \frac{\partial}{\partial x_j} \left( \sigma_k \frac{\partial k_p}{\partial x_j} \right) + G_p - \frac{\rho_p k_p^{3/2}}{\Lambda}
\] (II-1)
\[ \frac{Dk_T}{Dx_j} = \frac{\partial}{\partial x_j} \left( \frac{\nu_T}{\partial k} \frac{\partial k_T}{\partial x_j} \right) + \frac{\rho k_p}{\lambda} - \rho \varepsilon \]  

\[ \frac{D\varepsilon}{Dx_j} = \frac{\partial}{\partial x_j} \left( \frac{\nu_T}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) + \frac{1.08 \rho k_p}{\lambda^2 k_T} - C_2 \rho \varepsilon^2 \]

where \( G_p \) is the production term of turbulence kinetic energy:

\[ G_p = \nu_T \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial z} \right)^2 + \frac{\partial w}{\partial z}^2 + \frac{\partial u}{\partial r}^2 + \frac{\partial v}{\partial z}^2 \]

The turbulent viscosity in this model was expressed by:

\[ \nu_T = 0.078A \left( k_p + k_T \right) / \sqrt{k_p} \]

\( \lambda \) in the above equations was called the macroscale of turbulence, and was given as \( 0.14D_1 \) as an approximation(14).

The agitator boundary conditions were obtained from an implicit trailing vortex model, developed for describing the velocity profiles and turbulence parameters in the discharge stream(14). The details of this model for impeller stream will be discussed in a subsection later. In addition to provide three velocity components, this model also provided an estimate for \( k \) and \( \varepsilon \) at \( r=1.08R \), which was treated as the boundary instead of the impeller tip (\( r=1.0R \)). In their simulation they assumed that \( k_T \) at \( r=1.08R \) is insignificant and \( k_p \) is equal to \( k \) at \( r=1.08R \). In its adjacent regions, say, \( r=1.0R \) or \( r=1.1R \), \( k_p \) was specified, but \( k_T \) was not specified to be equal to the values at \( r=1.08R \). It implied that transfer eddies do not exist at \( r=1.08R \), but exist at \( r < \) or \( > 1.08R \). They also assumed the symmetry with the impeller plane and took only the top half of the vessel as their calculation domain. In addition, they specified values for
variables in the blade-swept region except for $k_T$ and $\varepsilon$, and thus this region was not included in the calculation, and they did not perform the material balance in this region.

The two-dimensional momentum equations along with the two-scale three-equation turbulence model were solved by using the method of stream function and vorticity transformations. As mentioned before, this method can not be expanded to a three-dimensional analysis.

Their predicted velocity profiles were compared with experimental data measured by a pitot tube only in the wall regions of the 0.294m diameter tanks with water as the fluid. The comparisons were made with the magnitude of theoretical and experimental resultant velocities instead of individual velocity components. Figures II-3 and II-4 show the comparisons of resultant velocity profiles near the tank wall for two different impeller speeds and diameters. The computed resultant velocity profiles were about 50% lower than the measured profiles. A qualitative comparison was made for the turbulence energy dissipation rates with the computer results of Placek(13) and Platzer(11). Placek, et al.(12) reported that only one order of magnitude difference of the dissipation rate in the bulk flow region was found in their simulation, while Placek(13) found one order of magnitude higher difference and Platzer(11) had two orders of magnitude higher.

In this model the production term for turbulence kinetic energy, $G_p$ in equation (II-4), only included three of the six components in this term for axisymmetrical flow. The production term is usually a dominant term in the turbulence energy equation, and omitting part of this term could lead to significant errors. For the limiting case of $k_T$ approaching zero, we find the second term in the right side of equation (II-3) will approach infinity. For the other limiting case with $k_p$ approaching 0, i.e., the
Figure II-3. Comparison of resultant velocity at the tank wall for $N = 400 \text{ min}^{-1}$ and $D_1 = D_i/3$ from Placek, et al. (12)
Figure II-4. Comparison of resultant velocity at the tank wall for $N = 840 \text{ min}^{-1}$ and $D_1 = D_T/4$ from Placek, et al. (12)
large-scale convective vortices disappeared and all the energy of large vortices had already been transferred into the small transfer or dissipation eddies. Thus, $v_t$ in equation (II-5) will approach infinity. Consequently, equation (II-5) is not universal to the entire flow region.

The motivation for the research of Placek, et al. (12) was to obtain a better description of the flow by extending the k-\(\varepsilon\) model to include the larger eddies generated by the vortices from the impeller tip with the small eddies. The comparison of their results obtained from the three-equation model (12) and the standard k-\(\varepsilon\) two-equation model (13) was not reported. The solution from this simulation was used by Smith (4, Chapter I) to study the dispersion and droplet phenomena in stirred vessels.

2.2.2 Analytical Tank Region Simulation

In this section, the three analytical tank region simulations will be reviewed. An analytical tank region simulation is defined as applying analytical solutions for the turbulent flow to regions of the tank such as impeller stream.

Six-Region Model by DeSouza and Pike (15):

DeSouza and Pike (15) made the first attempt to simulate the turbulent flow throughout the whole baffled mixing tank. They divided the baffled mixing tank into six regions, and used classical fluid dynamics solution to describe the flow in each region. In Figure II-5, one of their computer drawn solutions depicted the streamlines in the tank. Flow went from one region to another in the six regions. They were:

I. The discharge flow, modeled as a tangential jet.
Figure II-5. Typical computer drawn solution of flowfield with six regions from DeSouza and Pike(15).
II. The impeller stream approaching the tank wall, modeled as stagnation flow.

III. Upper and lower corners of the tank, modeled with the potential flow theory in a corner.

IV. Flow at the top and bottom of the tank away from the wall, also modeled by potential flow in a corner.

V. Flow at the center of the tank, modeled as a circular jet.

VI. Two doughnut-shaped elements, modeled as dead water regions.

In region I, an explicit tangential jet model, modified from the implicit one proposed by Nielsen(16), was derived and found to accurately describe the impeller stream as shown in Figure II-6 (15, Chapter I). The details of tangential jet models will be discussed in the next subsection. The potential flow theory, previous used by Larson(17) to describe the flow in the bulk of the tank, was applied to regions II, III and IV. Schlichtling's solution(18) for a circular jet in turbulent flow was used to describe the flow in region V.

The comparison of computed and experimental velocities was hampered by the accuracy of the three-dimensional pitot tube in regions II-IV where the velocities were smaller than the impeller region. Consequently, the comparison showed only qualitative agreement in parts of these regions. More significant was the observation that for most parts of the tank the tangential velocity components were of the same order of magnitude as two other velocity components. Their idea of segmented regions was adopted by other researchers(9,19).
Figure II-6. Comparison of velocity profiles in the impeller stream by DeSouza (15, Chapter I).
Four-Region Model by Desouza and Pike(15):

Desouza and Pike(15) extended the four-region analytical simulation of Desouza and Pike(15) to seven regions, which are shown in Figure 11-7 and listed below:

I-IV. Same as regions I-IV in the Desouza and Pike(15).

V. Flow at the center of the tank between the impeller and region IV. This is almost the same as regions V and VI of the Desouza and Pike's model(15).

VI. Flow in the region swept by the impeller.

VII. Flow at the top and bottom layer of the tank.

The classical solutions of Desouza and Pike(15) were adopted by Desouza and Pike(15) to describe the fluid flow in their first five regions. In the region VI, they assumed the streamlines were parallel to the impeller centerline in part of the blade-swept region, as used by Cooper and Wolf(20). Region VII was modeled as fully-developed boundary layer flow over a flat plate. Most of parameters in this seven-region model were from Desouza and Pike(15), and others were calculated from the data of Gunkel and Weber(7).

They showed that the tangential jet model overestimated the radial velocity in the impeller stream when compared with the experimental data by Sachs and Rushton(21). They also showed that outside the impeller region the deviation between the computed and measured axial velocities was as much as 100%.

Eight-Region Model by Fort, et al.(9):

Following the theoretical work by Desouza and Pike(15) and Desouza and Pike(15), Fort, et al.(9) again used a tangential jet model to describe
Figure II-7. Distribution of seven regions in stirred tanks(19).
the jet stream flow, and applied the assumption of the two-dimensional irrotational flow in the rest of the tank. They divided the tank into eight regions above and below the impeller plane. The segmented regions, shown in Figure II-8, can be described as follows:

I. Discharged jet from the impeller, modeled by the tangential jet proposed by DeSouza and Pike(15).
II. Stream impinging upon the tank wall, and changing the direction from radial to upward axial and downward axial.
III. Predominant axial velocity components at the tank wall.
IV. Upper and lower corner of the tank, in which velocity directions changed from axial to radial.
V. Predominant radial flow at the top and bottom layer of the fluid in the tank.
VI. Similar to II and IV, flow changing direction and both radial and axial components playing in the same role.
VII. Prevailing axial velocity components at the impeller axis.
VIII. Dead water region.

This eight-region model just re-divided the tank differently from DeSouza and Pike(15) and Ambegaonkar, et al.(19). The tangential velocity components were still treated as if they did not exist in the tank. In fact, the three velocity components are affected by each other, and thus they should be considered simultaneously. No comparisons for velocity profiles has been reported.

2.2.3 Tangential Jet Model and Trailing Vortex Model

As mentioned in Chapter I, the turbulent flow in agitated vessels is generated by a rotating impeller. This discharged stream from the
Figure II-8. Distribution of eight regions in stirred tanks(9).
impeller is particularly important. To describe the impeller stream, two different approaches have been developed: one is called tangential jet model, and the other one is trailing vortex model.

**Tangential Jet Model:**

Nielsen (16) made the first attempt to simulate the high velocity stream from the Rushton turbine using tangential jet. He time-averaged the equations of motion and simplified them with the boundary layer assumptions. He used Prandtl's mixing-length for eddy viscosity. By performing a similarity transformation, Nielsen (16) obtained an ordinary equation. From this transformed ordinary equation and continuity equation, the velocity profiles in the impeller stream can be obtained implicitly. The details of analytical solution are given in Nielsen's thesis (16).

Since Nielsen's jet model is implicit, it is inconvenient to be applied to obtain flow patterns in the discharge flow. Based on Nielsen's effort, DeSouza and Pike (15) then developed a three-parameter explicit tangential jet model as follows:

\[
V = V_{\text{max}}[1 - \tanh^2(n/2)] \\
U = -\frac{V_{\text{max}}}{\sigma} \left[ (\frac{2r^2 - a^2}{x^2 - a^2}) \tanh(n) - n(1 - \tanh^2(n/2)) \right] \\
W = V \tan \theta_y
\]

where

\[
V_{\text{max}} = \frac{1}{2} A (\sigma/r^2)^{1/2} (r^2-a^2)^{1/8}
\]

\[
n = \sigma z/r
\]

\[
\theta_y = \tan^{-1} \left( a/\sqrt{r^2-a^2} \right)
\]
The three parameters in this explicit model, i.e., \( \sigma \), \( a \) and \( A \), were given by (15, Chapter I):

\[
\begin{align*}
\sigma &= 12.621 \\
a &= 0.06924 \frac{(D_T - D_I)}{D_T} \\
A &= 1.1436 \left[ \frac{N D_I^3}{(R^2 - a^2)^{1.2}} \right]^{0.8377}
\end{align*}
\]

The above correlations were obtained from Cooper's (22) data for air and water and DeSouza's (15, Chapter I) data for water with various impeller speeds and diameters. The accuracy of this explicit version of tangential jet model was also established with the data for two different sizes of turbines by Drbohlav, et al. (23).

**Trailing Vortex Model:**

Van't Riet, et al. (24, 25, 26) concentrated on the flow between the turbine blades and the flow leaving the turbine blade tips. The velocity distributions were measured by photographs taken with a camera rotating at the same speed as the turbine impeller. He found that there were two symmetrical roll vortices on the rear side of the turbine blades. One was above and the other was below the impeller plane. The schematic view of this phenomena is shown in Figure II-9.

To describe the trailing vortex motion around the tip of the impeller, Van't Riet and Smith (24) used a circular cylindrical coordinate system with the origin located at the outer edge of the blade. Thus, the coordinate system used was rotating with the impeller blade tip. They proposed to use simplified Navier-Stokes equations in the rotating coordinate system and the continuity equation to describe the velocity and pressure distribution within the trailing vortex.
Figure II-9. Schematic 3-D view of the trailing vortex pair behind each impeller blade (Top), and 2-D view of the flow field in the impeller region. S, stagnation point after Van't Riet and Smith(24).
To solve this set of equations, Van't Riet and Smith (24) used a different approach to solve for velocity components. First, they obtained an empirical equation for axial velocity based on experiments. Then they could analytically derive an equation for radial velocity from the continuity equation. Before incorporating these two velocity components into their Navier-Stokes equation, they made two assumptions: first, the eddy viscosity is constant; and second, the z-gradient of the circumferential velocity of trailing vortex is zero. Then their Navier-Stokes equation for the circumferential velocity within the trailing vortex can be solved. There were three parameters in this model which were determined by experiments.

A major achievement in Van't Riet and Smith's (24) trailing vortex model is that they established an axis system for the trailing vortex and obtained an empirical equation to estimate the vortex rotational speed. However, they started their model development by obtaining an expression for axial velocity from experiments. The validity of this vortex model was influenced by the accuracy and universality of this expression. Besides, the assumption of constant effective viscosity, which is sum of molecular and turbulent viscosity, made their analytical solution possible. Unfortunately, they admitted this was inaccurate (24). No comparison for computed and measured radial velocity was reported. This model was validated by only one graph for the vortex circumferential velocity with an error of as high as about 50%.

A disadvantage of this vortex model is that it did not provide an expression for the tangential velocity component based on the stationary cylindrical coordinate system. Therefore, this model is inconvenient for use.
Placek and Tavlirides(14) started from the concept of the rotating coordinates by Van't Riet and Smith(24) to obtain a stationary trailing vortex model on the cylindrical coordinate system. After a complicated transformation, they developed a 13-equation model for the three velocity components. One of these equations in this stationary trailing vortex model needed to be solved implicitly. Thus, this vortex model is implicit. Since the Van't Riet and Smith's(24) formula for the circumferential velocity within the trailing vortex was not accurate, they used interpolated values from experiments for this rotational vortex velocity in their model. This increased the difficulty to utilize this model. Then, based on the experimental data by Gunkel and Weber(7), Placek and Tavlirides(14) also developed estimation for turbulence kinetic energy and dissipation rate. As discussed before, this model was used to provide boundary conditions at impeller tip in a two-dimensional numerical simulation for the turbulent flow in an agitated vessel(12).

The calculated axial profile of resultant mean velocity at r=1.09R was compared with Gunkel and Weber's(7) data. The discrepancy near the impeller plane was about 10%, but the difference at the turbine blade edge was more than 100%.

It should be pointed out that a couple of trailing vortices were discovered by Van't Riet and Smith(24,25,26) and Van Der Molen, et al.(27). However, Gunkel and Weber(7) observed four vortices behind the turbine blade. Placek and Tavlirides(14) did not report that how many trailing vortices can be obtained from their vortex model, even though they have transformed the velocity components back to the vortex rotational velocity on the rotating coordinate system set by Van't Riet and Smith(24).
We then will select a model for the impeller boundary conditions in our
umerical simulation based on a practical viewpoint. Placek and
Tavlarides(14) did not compare the tangential jet model and trailing
vortex model. Their stationary trailing vortex model is implicit and
involves 13 equations with one variable needed to be incorporated from
experiments. Thus, this vortex model is not practical. As for the
explicit tangential jet model by DeSouza and Pike(15), we find it is the
easiest model to be applied to the flow in the region close to the
impeller. Consequently, the tangential jet model will be used in our
research.

2.3 Experimental Studies

There have been a number of experimental studies on various aspects of
the turbulent flowfield in baffled stirred tanks. They include
measurements of mean velocity and turbulent properties.

Velocity Profiles in the Bulk Region by Mulvahill(6, Chapter I):

Parikh(7, Chapter I) and Khungar(8, Chapter I) demonstrated that a hot
wire anemometer could be used to measure the turbulent velocity profiles
of a 5 centistokes non-conducting silicone fluid in an agitated vessel.
Then Mulvahill(6, Chapter I) refined their measurements using a specially
designed three-wire probe to measure the mean velocity components in the
same silicone fluid outside the impeller stream. Measurements were taken
for three different impeller speeds (150, 200 and 250 rpm) and two
different size Rushton turbines (3 and 4 inches) in a 11.5 inches diameter
stirred tank conformed to the standard tank configuration. Table II-1
compares his tank configuration to that of the standard tank. The
Table II-1. Standard versus Actual Tank Configuration Used by Mulvahill (6, Chapter 1)

<table>
<thead>
<tr>
<th></th>
<th>Standard Tank Configuration</th>
<th>Configuration with 4-inch impeller</th>
<th>Configuration with 3-inch impeller</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Height</td>
<td>$D_T$</td>
<td>$D_T$</td>
<td>$D_T$</td>
</tr>
<tr>
<td>Impeller Diameter</td>
<td>$D_T/7$ to $D_T/2$</td>
<td>$D_T/2.9$</td>
<td>$D_T/3.8$</td>
</tr>
<tr>
<td>Number of Turbine Blades</td>
<td>6</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Distance from Turbine to Tank Bottom</td>
<td>$D_I$ to $2.5D_I$</td>
<td>$1.4D_I$</td>
<td>$1.9D_I$</td>
</tr>
<tr>
<td>Impeller Diameter : Blade Length</td>
<td>20 : 5 : 4</td>
<td>20 : 5 : 4</td>
<td>20 : 5 : 4</td>
</tr>
<tr>
<td>: Blade Width</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of Baffles</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Baffle Width</td>
<td>$D_T/10$ to $D_T/12$</td>
<td>$D_T/11.5$</td>
<td>$D_T/11.5$</td>
</tr>
</tbody>
</table>
Reynolds number for the flow in the tank was 4,840 for 3-inch impeller at 250 rpm and 5,160 and 6,880 for 4-inch impeller at 150 and 200 rpm.

Figure II-10 shows the profiles of axial velocity components on the 45° plane in the stirred tank system with a 3" turbine rotating at 250 rpm. Figure II-11 shows the profiles of tangential velocity components along the tangential direction in three different tank systems. Mulvahill (6, Chapter I) found the velocity profiles were not symmetrical above and below the centrally located impellers. A total of 78 positions in the three tank systems was used by Mulvahill for velocity measurements. The resulting velocity profiles were claimed to be consistent and reproducible to within 5% (6, Chapter I). The accuracy of the profiles was also verified by comparing the tank circulation rates, obtained from the integration of the velocity distribution along the tank wall, with the circulation rates based upon entrainment into the impeller stream (6, Chapter I). Therefore, his experimental data will be used for the validation of the velocity profiles computed in this work.

Turbulence Energy Dissipation Rates in the Jet Stream by Patterson and Wu (28):

Patterson and Wu (28) used a laser Doppler velocimeter to obtain the values of the dissipation rates of the turbulence energy in the jet zone. Three impeller rotation speeds were used which were 100, 200 and 300 rpm for a 27 cm diameter tank with a 9.3 cm turbine and water as the fluid. They found that the turbulence in most locations of this region was not strongly nonisotropic, and thus they concentrated their measurements near the impeller tip where the nonisotropic jet was discharged. Figure II-12 shows measurements of the distribution of turbulence energy dissipation rates for three different impeller rotation speeds. It was observed that
Figure II-10. Axial velocity components on the 45° plane in the tank with 3" turbine at 250 rpm from Mulvahill (6, Chapter I).
Figure II-11. Angular velocity components along the θ-direction in three tank systems from Mulvahill (6, Chapter I).
Figure II-12. Normalized turbulence energy dissipation rates in the impeller stream from Patterson and Wu(28).
the effect of the impeller speeds was small on the normalized dissipation rates, $\varepsilon/\rho N^2 D_i^2$ as shown in Figure II-12. The largest effect was at $r/R = 1.0$ and at $z/R = 0$, i.e., at the impeller tip. The differences caused by the rotation speeds were shown to occur on the impeller plane where the values of the nondimensionalized dissipation rates are the highest. At $r/R = 1.72$ the differences disappear and the curves become flatter. According to Patterson and Wu(28), these phenomena implied that most power consumption occurred in the jet zone, especially close to the impeller tip.

Flow Phenomena by Gunkel and Weber(7):

A comprehensive study of the flow phenomena of air in mixing tanks with a Rushton turbine was done by Gunkel and Weber(7). They used a shielded hot-wire anemometer to obtain mean velocities, fluctuating components, energy spectra, and energy dissipation in the entire tank. This study employed a 45.7 cm diameter tank with a 22.8 cm turbine at 200, 400 and 600 rpm.

They found that velocity profiles in the impeller stream showed a turbulent jet behavior with entrainment as discussed previously. Also, four vortices were reported from between each pair of blades: two above and two below the disc. This is twice the number observed by Van't Riet and Smith(24) and Van Der Molen, et al.(27). In addition, their results showed a large radial flow outward from behind the blades and lower radial velocity in the front face of the blades which agreed with what Van't Riet, et al.(24,25) had obtained.

Gunkel and Weber(7) also found the fluctuating velocity has a strong periodic component near the impeller blades. Measurements between the impeller blades indicated that the root mean squared (r.m.s.) fluctuating
velocity is almost independent of the position. They also found that random fluctuations in the impeller region were small. The strong random fluctuations observed in the region close to the blades might be due to the vortices formed inbetween the blades. This is the same conclusion as Van't Riet, et al.(24,25).

Based on the velocities obtained in the impeller region, Gunkel and Weber(7) estimated the energy dissipation rate in the tank by performing an energy balance on a control volume containing the impeller. They claimed that most of the impeller power is dissipated in the bulk region of the tank. This conclusion was contradictory to other works, e.g., Patterson and Wu(28).

In the bulk region of the tank, Gunkel and Weber(7) observed that the resultant mean flow is essentially in the axial direction. They inserted the probe from the top of the tank with the direction parallel to the mean flow vector to measure the tangential and radial components, and they found their data for these two velocity components are not as reliable as the axial velocity components. The r.m.s. velocities were found not to differ much from one position to another. Thus, they concluded that an approximate isotropic and homogeneous turbulence for the flow may be acceptable.


Bertrand, et al.(29) used a hot film anemometer to measure the flow parameters in the discharge jet from five different radial flow impellers in a 40 cm diameter tank with water as a fluid. They assumed the axial velocity was zero in the stream, and measured the other two velocity components. Jet-like behaviors were observed from the bell-shaped curves of the profiles for both radial and tangential velocity components in the
axial direction. They considered the existence of the angle profile with
which the discharge flow leaves the blade tips, and proposed to determine
it by taking $\tan^{-1}$ of the ratio of the mean tangential velocity to the
mean radial velocity. The calculated results showed that the angle
profile was a constant, which is different for the various impellers.

Bertrand, et al. (29) also obtained the pumping capacities for the five
different impellers. Their results illustrated that the discharge flow
rate is proportional to the impeller speed, but the proportional constant
is different for various impellers. They found that the pumping capacity
decreases when the blade width decreases, and increases when the impeller
is lowered from the midway of the tank.

The r.m.s. fluctuating velocities in three directions were also
determined. A comparison among them showed that the turbulence was not
isotropic in the jet zone for all five impellers. The data also showed
that the radial and tangential turbulence intensities were complicated
functions of $z$, and no simple correlation could be found.

Turbulence Measurements in the Impeller Stream by Mujumdar, et al. (30):

A constant temperature hot-wire anemometer was used to measure the mean
and fluctuating velocities near a 5" and 6" turbine in a covered and
baffled 15" diameter mixing tank filled with air. Mujumdar, et al. (30)
found that a local maximum for r.m.s. velocity distribution occurred in the
radial direction, but the mean values kept decreasing to the tank wall.
They reported that the local intensity of turbulence increased with $r$
since the mean velocity decreased in the $r$ direction more quickly than the
r.m.s. fluctuating velocity.
Turbulence Characteristics in the Impeller Stream by Rao and Brodkey(31):

Rao and Brodkey(31) measured velocities of the jet from a 10.2 cm turbine in a 29.5 cm diameter tank of water with four equally spaced baffles. Three-dimensional pitot tube was used first to determine the directions of the mean velocity vectors. Rao and Brodkey(31) found that the mean velocities obtained with the pitot tube were much higher than those with the hot film anemometer. They attributed this situation to the fact that for a high intensity and large scale turbulence in the stream, the static pressure registered by a pitot tube is lower than the true value of static pressure; thus erroneous outcomes were obtained with the pitot tube.

Then they adopted a constant temperature hot film anemometer to determine the magnitude of the velocities and the turbulence parameters, e.g., turbulence intensities, in the direction of the velocity vectors which was similar to the works of Mujumdar, et al.(30). The turbulence field was found to be anisotropic and intermittent, the latter being caused by a strong turbulent jet from the impeller. The presence of periodic velocities close to the impeller was also observed. Although anisotropy was detected, Rao and Brodkey(31) used an isotropic relationship to estimate the dissipation of the turbulence energy.


In addition to the study of velocity profiles near the impeller tip which has been previously discussed, Van't Riet, et al.(24) used a stationary conical hot film anemometer probe for turbulence measurements of the vortex motion. Because of the dominant existence of vortices in the impeller discharge, they said that, when local velocities are determined with a stationary probe, the vortex sweeping along the probe
may generate a considerable non-random pseudo-turbulent fluctuations. Thus, true turbulence parameters, such as eddy size, turbulent intensity and energy spectra, cannot be determined simply from velocity measurements with a stationary probe in the jet stream. They pointed out that the macroscale of turbulence as determined by Mujumdar, et al.(30) and Rao and Brodkey(31) is of the magnitude of the diameter of the vortex. Since the energy dissipation scales are significantly affected by the above-mentioned pseudo turbulence, Van't Riet, et al.(24,25) thought the calculated local energy dissipation rates near the impeller are certainly too high. They also considered that the true turbulence parameters can be determined by a stationary probe only in the bulk region, since the vortices are broken up when they reach the baffles and tank walls. They felt that real turbulence measurements in the impeller region can only be made with a probe rotating with the impeller.

Flow Study in the Impeller Region by Van Der Molen, et al.(27):

Van Der Molen, et al.(27) declared that it was impossible to measure flows in stirred tanks because of significant disturbances by probes and their supports until the development of the laser Doppler velocimeter. They used a laser Doppler velocimeter, equipped with a frequency shift in order to eliminate the ambiguous measuring direction, to study the turbulent flow in the turbine impeller region of stirred vessels containing water. They reported that, like Van't Riet and Smith(24), one pair of counter-rotated vortices formed inbetween the blades and dominated the region $1 \leq r/R \leq 1.5$. The non-dimensionalized circulation velocity in the vortices was found to be very sensitive to the geometry, and to increase with scale-up. The mean velocity in the jet stream was reported to be proportional to the impeller tip speed. Van Der Molen, et al.(27)
also said that due to entrainment the radial velocity increased in proportion to \((r/R)^{-7/6}\). They failed to consider the turbulence intensity in the \(\theta\)-direction, and they concluded that the turbulent flow in the impeller region was isotropic. This is contrary to Bertrand, et al.(29) and Rao and Brodkey(31).

**Velocity Profile in the Top Half of the Tank by Nagata and Associates(4,32,33):**

It is believed that one of the earliest and most comprehensive work on the measurements of mean velocity profiles for various configurations of the mixing tank was made by Nagata and associates. Their research was presented in two articles(32,33) and summarized in Nagata's book(4). In their research, water was used as the fluid, and the impeller was an eight-flat-blade turbine centrally located in the tank which had eight baffles. Therefore, Nagata's tank configuration is different from the standard tank configuration. Nevertheless, their results can still help us to understand how the liquid may flow throughout the tank while agitated by an impeller.

Nagata used pitot tubes to measure the velocity profiles for high Reynolds numbers and used a photographic method for low Reynolds numbers in the top half of the tank. They reported that the flow was rapidly discharged from the impeller and flowed upwards quickly in the space close to the tank wall. Then the flow turned over and pointed back down into the impeller region. Consequently, they made a conclusion that the insertion of baffles reduces the tangential component of the fluid velocity and increases the other two velocity components by causing the flow to turn in the axial direction.
Velocity Profiles Near the Impeller by Sachs and Rushton(21):

Sachs and Rushton(21) did the first quantitative study of the flow in the neighborhood of a 4" six-flat-blade turbine by measuring velocities at five radial positions with the photographic method in a 12" diameter tank with water as the fluid. The radial velocity profiles in the impeller stream were observed to be bell-shaped, and tended to flatten as the flow moved from the impeller tip to the tank wall. The volumetric flow rate discharged from the impeller was found to be proportional to the impeller speed. In addition, the volumetric flow rate from the impeller increased with the radial distance because the impeller stream entrained the adjacent fluid.

They also observed that the radial velocity distribution between the impeller blades reached a maximum at 50° ahead of the indexed blade and was 38% higher than the average value. This experimental result showed the oscillatory effect of the impeller, and this pulsating phenomena of the radial velocity component was observed to extend from the impeller shaft to a location equal to \((2/3)(D_T/2)\). Also, it was reported that the fluid leaves the impeller at an angle of 53°. This meant there was a tangential velocity at the periphery of the impeller.

Other Studies:

In addition to the experimental studies mentioned above, there have been some other related studies worth mentioning. Weetman and Salzman(34) studied the effect of side flow on the fluid behavior in mixing tanks. They used the laser Doppler velocimeter to obtain velocity vectors for both axial and radial type of impellers. Aiba(35) used the radioisotope of cobalt as a means of measurement to obtain the velocity profiles of water and glycerine solutions as fluids in the unbaffled and baffled tanks.
equipped with three representative types of impellers, namely propeller, turbine and paddle. Cutter(36) used the photographic method and Kiel impact tube to measure mean and fluctuating components of velocity of water in a stirred tank. Metzner and Taylor(37) used the photographic technique to measure velocity distribution in both viscous Newtonian and non-Newtonian fluids agitated by a flat blade turbine in a baffled tank with rotation speeds ranging from 60 to 600 rpm. Cooper and Wolf(38) studied the velocity profiles for the turbine type impellers by using a hot wire anemometer and the two- and three-dimensional pitot tubes in both air and water. Pumping capacities were then calculated from these velocity distributions. Holmes, et al.(39) obtained the velocity distributions around the impeller plane by measuring the response to a pulse of ionic tracer injected into the impeller region with a conductivity cell around the impeller. From these velocity results they estimated the volumetric flow rate of water and glycerine in the radial direction. Askew and Beckmann(40) used an impact tube which extended through the wall to measure the velocity components at the tank wall. Kudrna, et al.(41) concentrated their measurements of velocity in the neighborhood of the tank bottom by using a modified three-opening pitot tube method.

2.4 Summary

A comprehensive review of the previous works on the velocity profiles and related phenomena of the fluid dynamics in a baffled stirred vessel has been presented. There has been a significant amount of experimental work which helps to qualitatively describe the flow in stirred tanks. For example, the impeller stream can be described as tangential jet. However,
there have been limited measurements of turbulence parameters in the impeller region and the rest of the tank. More experiments are needed to illuminate the turbulent phenomena in a mixing tank.

There have been seven studies on the description and prediction of the flow behavior in the entire mixing tank. Three of them combined classical fluid dynamics models. In these three studies, the impeller stream was treated as a tangential jet and the flow in the bulk of the tank was assumed as a two-dimensional irrotational flow. However, experimental measurements have shown that the actual flow in the baffled mixing vessels is three-dimensional with the three velocity components being of the same order of magnitude. The tangential velocity component must not be neglected, even though axisymmetry is assumed, i.e., all θ-gradients are negligible.

The other four studies solved the equations of motion and the turbulence model numerically. Using the standard k-ε turbulence model, Middleton, et al.(5, Chapter I) applied the finite domain method to obtain a three-dimensional solution. However, he did not report the validation of his solution. Harvey and Greaves(6) used the same method as Middleton, et al. and Platzer(11) used the stream function and vorticity transformations to solve the two-dimensional Navier-Stokes equations with the classic k-ε turbulence model. Their results showed that the classic k-ε model is not suitable for the turbulent flow in baffled agitated vessels. Placek, et al.(12) split the standard k-equation into two equations, and thus formed a three-equation turbulence model. With this modification they made their two-dimensional solution. Their two-dimensional computer code was based on the method of stream function and vorticity transformations. They did not compare their turbulence model with the classic model used by other studies.
The values of velocity components at the impeller tip are required as the boundary conditions for the momentum equations, and we have carefully reviewed the two analytical approaches to describe the flow leaving the turbine blades. These are the tangential jet model and trailing vortex model. We have determined that the tangential jet model is the appropriate one to calculate the velocity components at the impeller tip.

In summary, a reliable three-dimensional simulation is still required to describe the fluid dynamics phenomena in a mixing tank. As a contribution, this work will obtain a simulation to describe the three-dimensional turbulent flow in baffled stirred tanks.
2.5 References


3.1 Introduction

In this chapter, the equations governing the turbulent fluid motion in an agitated vessel are developed, and their numerical solution is given. A turbulence model, a necessity for closing the Navier-Stokes equations, can be regarded as the crux of the description of the turbulent motion in a baffled mixing tank, and thus is central to a precise description of the flow. The discrete form of the governing equations will be described in detail, and then a well-known solution procedure and its revised version of dealing with the non-linearity of the continuity equation and the pertinent transport equations will be discussed. These solution procedures were adopted because of their flexibility with both two- and three-dimensional transport equations, e.g. Navier-Stokes equations, energy equation, species continuity equations, and equations for turbulent quantities; all of which are simultaneously interlinked with each other to characterize the complexity of a non-reacting or reacting flow system. Finally, the special boundary conditions for the impeller-driven flows will be discussed and be written in appropriate forms for numerical solutions. The material presented in this chapter formed the basis of a computer code which was used to obtain the numerical solution of the turbulent transport equations.
3.2 Conservation Equations for Turbulent Flows

As pointed out in the previous chapters, the fundamental equations describing the fluid dynamics in a stirred tank are the differential equations of mass and momentum conservation. These conservation laws can be written as:

**Continuity:**  \[ \frac{Dp}{Dt} = -\rho \nabla \cdot \mathbf{V} \]  (III-1)

**Momentum:**  \[ \rho \frac{D\mathbf{V}}{Dt} = -\nabla p - \rho \nabla \mathbf{t} + \rho g \]  (III-2)

Let \( V_r, V_\theta, \) and \( V_z \) be the three components of the velocity vector \( \mathbf{V} \) in cylindrical coordinates. The above equations can be written in this coordinate system for an incompressible Newtonian fluid as follows:

**Continuity:**

\[ \frac{1}{r} \frac{\partial}{\partial r} (rv_r) + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z} = 0 \]  (III-3)

**Momentum:**

- **r-component** --

\[ \rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + \frac{v_z}{r} \frac{\partial v_r}{\partial z} \right) = -\frac{\partial p}{\partial r} + \mu \left( \frac{1}{r} \frac{\partial (rv_r)}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_r}{\partial \theta^2} - \frac{2}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z} \]  (III-4)

- **\( \theta \)-component** --

\[ \rho \left( \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_z}{r} \frac{\partial v_\theta}{\partial z} \right) = -\frac{1}{r} \frac{\partial p}{\partial \theta} + \mu \left( r \frac{\partial (rv_\theta)}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_\theta}{\partial \theta^2} + \frac{2}{r} \frac{\partial v_r}{\partial \theta} + \frac{\partial v_z}{\partial z} \]  (III-5)
For turbulent flow, the instantaneous velocity components and pressure can be replaced by the sum of a time-averaged component and fluctuating component as given below.

\[
\begin{align*}
\bar{V}_z &= V + v \\
V_r &= V + v \\
V_\theta &= W + w \\
V_z &= U + u
\end{align*}
\]

In equation (III-7), the capitals in the right hand side represent time-averaged values, and the small symbols stand for the fluctuating quantities of the turbulent flow.

Substituting the quantities of equation (III-7) into the equations of motion, equations (III-3) to (III-6), and performing the time-averaging procedure(1), the Reynolds equations of motion for the steady incompressible turbulent flow in agitated vessels become:

\[
\begin{align*}
\frac{1}{r} \frac{\partial (rV)}{\partial r} + \frac{1}{r} \frac{\partial W}{\partial \theta} + \frac{\partial U}{\partial z} &= 0 \\
\rho \left( \frac{\partial (V^2)}{\partial t} + \frac{1}{r} \frac{\partial (rW)}{\partial \theta} - \frac{W^2}{r^2} + \frac{\partial (UV)}{\partial r} + \frac{V^2}{r} \right) &= - \frac{\partial P}{\partial r} + \mu \left( \frac{1}{r} \frac{\partial (rV)}{\partial r} + \frac{1}{r^2} \frac{\partial V}{\partial \theta} \right) + \frac{1}{r^2} \frac{\partial ^2 V}{\partial \theta ^2} \\
&- 2 \frac{\partial W}{r} \frac{\partial V}{\partial \theta} - \frac{\partial ^2 W}{\partial z ^2} - \rho \left( \frac{\partial ^2 V}{\partial r ^2} + \frac{1}{r} \frac{\partial (rV)}{\partial \theta} - \frac{W}{r} + \frac{\partial (UW)}{\partial r} + \frac{V}{r} \right)
\end{align*}
\]
In these equations the bar over the product of the fluctuating components indicates the time-averaged quantities. Six dependent variables associated with the fluctuating components, i.e., \( \overline{u^2}, \overline{v^2}, \overline{w^2}, \overline{uv}, \overline{vw}, \) and \( \overline{w^2} \), make these equations much more complicated than equations for laminar flow. For laminar flow, there are four differential equations for four unknowns, i.e., three velocity components and pressure; and it is said that a closure system is formed, i.e., the same number of equations as dependent variables. For turbulent flow, however, the closure problem arises because there are more dependent variables than differential equations, as shown in equations (III-8) to (III-11). A separate description of the time-averaged products of the turbulent fluctuation is required, and closure or turbulence models are used. The mathematical expressions for these turbulent stresses are the subject of next section.

The two-dimensional form of the conservation equations comes from assuming symmetry about the \( \theta \)-coordinate and is an approximation if the turbine impeller is centrally located in a cylindrical vessel. Thus, the terms involving \( \partial^2 / \partial \theta^2 \) and \( \partial^2 / \partial \theta^2 \) in the three-dimensional governing equations can be deleted. However, the terms including \( W \) and \( w \) are
retained because the tangential velocity $V_\theta$ exists in the agitated vessel. The two-dimensional differential equations for the turbulent flow can be written as follows:

\[
\frac{1}{r} \frac{\partial(rV_r)}{\partial r} + \frac{\partial u}{\partial z} = 0 \quad (III-12)
\]

\[
\rho \left[ \frac{\partial (V^2)}{\partial r} - \frac{u^2}{r} + \frac{\partial (UV)}{\partial z} \right] = - \frac{\partial p}{\partial r} + \nu \left( \frac{1}{r} \frac{\partial (rU)}{\partial r} - \frac{\partial V}{\partial z} \right) + \frac{\partial^2 U}{\partial z^2} - \rho \left[ \frac{\partial (U^2)}{\partial r} - \frac{u^2}{r} + \frac{\partial (UU)}{\partial z} \right] \quad (III-13)
\]

\[
\rho \frac{\partial (W)}{\partial r} + 2 \frac{W}{r} + \frac{\partial (WU)}{\partial z} = \nu \left( \frac{1}{r} \frac{\partial (rW)}{\partial r} - \frac{\partial U}{\partial z} \right) + \frac{\partial^2 W}{\partial z^2} - \rho \left[ \frac{\partial (W^2)}{\partial r} + 2 \frac{W^2}{r} + \frac{\partial (WW)}{\partial z} \right] \quad (III-14)
\]

\[
\rho \frac{\partial (UV)}{\partial r} + \frac{\partial (V^2)}{\partial z} = \rho \frac{\partial Z}{\partial r} - \frac{\partial p}{\partial z} + \nu \left( \frac{1}{r} \frac{\partial (rU)}{\partial r} + \frac{\partial V}{\partial z} \right) + \frac{\partial^2 U}{\partial z^2} - \rho \left[ \frac{\partial (UV)}{\partial r} + \frac{\partial (U^2)}{\partial z} \right] \quad (III-15)
\]

The turbulent stress terms appearing in the above equations will be described with turbulence models as discussed below. Also, for convenience we will use the two-dimensional form of conservation equations in the following discussion. Then the three-dimensional form of the equations will be given as a direct extension of the two-dimensional equations.

### 3.3 Mathematical Models of Turbulence

When the instantaneous turbulent velocity components and pressure are expressed as the sum of mean and fluctuating components and the equations
of motion are time-averaged, we start with four dependent variables and end up with ten time-averaged unknowns (U, V, W, P, and six Reynolds stress components), as shown in last section. This is part of the closure problem of turbulence. If the time-averaged products of the turbulent fluctuations are considered statistical correlation functions, the equations of continuity and motion can be manipulated (2, 3) to give a tensor-form equation in terms of a second or a third order correlation functions, i.e., one equation and two unknowns. Further manipulations add another equation but with another higher order correlation. This procedure can be continued, but the result is \( n \) equations and \( n+1 \) unknowns. Thus, it is necessary to turn to models of the Reynolds stresses as one way to overcome this closure problem.

Early investigators employ Boussinesq's (1877) suggestion to express the turbulent stresses in Reynolds-averaged turbulent flow with the same form as that used for the laminar flow. According to Boussinesq, the turbulent stresses could be represented by the product of the mean-flow velocity gradients and a turbulent viscosity, \( \mu_t \). This viscosity is not a property of the fluid and will vary with positions in the turbulent flow. This is the simplest way to describe the turbulent stresses in the equations of motion.

The concept of using a turbulent viscosity to account for the turbulence effects continues today, even though the simple model of Boussinesq was inadequate. The task is to determine how to express the turbulent viscosity in terms of known or computable quantities of the flow. Different expressions for the turbulent viscosity provided different turbulence models. According to the classification made by Launder and Spalding (4), turbulence models in terms of the turbulent viscosity can be categorized into two groups. One is the algebraic models
where the turbulent viscosity is obtained by algebraic formulas, in which the only unknowns involved are the properties of the mean-flow velocity field. The other is the differential models where the turbulent viscosity comes from the solution of the differential equations for one or more properties of the turbulent flow. If one differential equation is to be solved for the turbulent viscosity, the closure is accomplished by a one-equation model. Closure models constructed from two differential equations are called two-equation models.

Generally the turbulent viscosity has been assumed to be isotropic. In an isotropic turbulence model, the six components of the turbulent viscosity are equal. An example of a two-equation isotropic turbulence model was given by equations (I-1,2) in Chapter I. In a nonisotropic turbulence model, the viscosity may have six different components. Lilley, et al.(5-8) developed a k-kL two-equation nonisotropic turbulence model for the free swirling jet.

In this study, one isotropic and one nonisotropic k-ε two-equation model is used to describe the turbulent flow in turbine-agitated vessels. The conservation equations associated with these two different closure models are presented in the subsequent subsections.

3.3.1 Isotropic Model

The turbulent equations of motion can be put in a form containing the turbulent viscosity by replacing the Reynolds stress terms with the product of the time-averaged velocity gradients and the turbulent viscosity. For axisymmetric two-dimensional flow in an agitated vessel, equations (III-13) to (III-15) become:
\[ \rho \left( \frac{1}{r} \frac{\partial}{\partial r}(r \nu r) + \frac{\partial}{\partial z}(U) \right) = \frac{1}{r} \frac{\partial}{\partial r}(r \nu r \frac{\partial}{\partial r} + \frac{\partial}{\partial z}(\nu r \frac{\partial}{\partial z} - \frac{\partial P}{\partial r} + \rho \frac{V}{r} - 2 \nu \frac{V}{r^2} + \frac{1}{r} \frac{\partial}{\partial r}(r \nu \frac{\partial}{\partial r} + \frac{\partial}{\partial z}(\nu \frac{\partial}{\partial z}) \right) \]  

\[ (\text{III-16}) \]

\[ \rho \left( \frac{1}{r} \frac{\partial}{\partial r}(r^2 U) \right) = \frac{1}{r^2} \frac{\partial}{\partial r}(r^3 U) + \frac{\partial}{\partial z}(\nu r \frac{\partial}{\partial z} - \frac{\partial P}{\partial z}) \]  

\[ (\text{III-17}) \]

\[ \rho \left( \frac{1}{r} \frac{\partial}{\partial r}(r U) + \frac{\partial}{\partial z}(U) \right) = \frac{1}{r} \frac{\partial}{\partial r}(r \nu \frac{\partial}{\partial r} + \frac{\partial}{\partial z}(\nu \frac{\partial}{\partial z}) - \frac{\partial P}{\partial z} + \rho g_z \]  

\[ + \frac{1}{r} \frac{\partial}{\partial r}(r \nu \frac{\partial}{\partial z} + \frac{\partial}{\partial z}(\nu \frac{\partial}{\partial z}) \right) \]  

\[ (\text{III-18}) \]

where the effective viscosity is the sum of the molecular and turbulent viscosities and is given by:

\[ \nu_{\text{eff}} = \mu + \nu_t \]  

\[ (\text{III-19}) \]

The effective viscosity \( \nu_{\text{eff}} \) is a function of position in the flowfield and is not a constant, so further simplification of equations is not possible.

According to Launder and Spalding(9), the standard k-\( \varepsilon \) two-equation model is considered to be more accurate than mixing-length models and one-equation models. In the k-\( \varepsilon \) model, the turbulent viscosity is determined from the solutions to the transport differential equations for the turbulence kinetic energy, \( k \), and its dissipation rate, \( \varepsilon \). These two turbulence parameters are defined as follows(10):

\[ k = \frac{1}{2}(u^2 + v^2 + w^2) = \frac{1}{2}u_i^2 \]  

\[ (\text{III-20}) \]
This model has been applied to the turbulent flow in agitated vessels (5, Chapter I; 6, 11, 12, Chapter II) as well as in other flowfields (9,11-19). The two-dimensional form of this $k$-$\varepsilon$ model in cylindrical coordinate is:

$$
\rho \left( \frac{1}{r} \frac{\partial}{\partial r} (r \rho v_k) + \frac{\partial}{\partial z} (\rho v_k) \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_{eff}}{\varepsilon} \frac{\partial \rho_k}{\partial r} \right) + \frac{\partial}{\partial z} \left( \frac{\mu_{eff}}{\varepsilon} \frac{\partial \rho_k}{\partial z} \right) + C_{1}\rho \varepsilon - C_{2}\rho \varepsilon \tag{III-22}
$$

where the generation term $G$ is

$$
G = \nu_t \left[ 2 \left( \frac{\partial V}{\partial x_i} \right)^2 + \frac{V_i^2}{x_i} \right] + \left( \frac{\partial V_j}{\partial x_i} \right)^2 + \left( \frac{\partial V_i}{\partial x_j} \right)^2 + \frac{\partial V_i}{\partial x} \frac{\partial V_j}{\partial x} \right] \tag{III-24}
$$

The turbulent viscosity $\nu_t$ is defined by the following equation (9):

$$
\nu_t = C_{\mu} \rho k^2 / \varepsilon \tag{III-25}
$$

The conservation equation for turbulence kinetic energy is obtained by multiplying each component of the momentum equations by the fluctuating velocity component in that coordinate direction, time-averaging the three equations and then adding them together to give equation (III-22) (4). The conservation equation for the energy dissipation rate is obtained by differentiating the equations of motion for $u_i$ with respect to $x_i$, multiplying through by $2\nu \partial u_i / \partial x_j$ and then rearranging to give equation (III-23) (3).

Launder and Spalding (4) recommend the following values for the coefficients appearing in the standard $k$-$\varepsilon$ model, i.e., equations (III-22, 23, 24, 25):

$$
\sigma_k = 1.0 \tag{III-26}
$$
$$\sigma_\varepsilon = 1.3 \quad (\text{III-27})$$
$$C_\mu = 0.9, \ C_1 = 1.44, \ C_2 = 1.92 \quad (\text{III-28})$$

Actually, the above set of coefficients is subject to change for various turbulent flows. For example, Harvey and Graves (6, Chapter II) used $\sigma_k = 0.9, \sigma_\varepsilon = 0.9, \text{and } C_1 = 1.43$ in their $k$-$\varepsilon$ model for the flow in agitated vessels. Also, Sonin (20) calibrated the $k$-$\varepsilon$ model parameter $\sigma_k$ using data from the experiments on the steady diffusion of turbulence made by Thompson and Turner (21) and Hopfinger and Toly (22). He used the values given in equations (III-27) and (III-28) and obtained $\sigma_k = 0.87$ with the data from Thompson and Turner (21) and $\sigma_k = 0.74$ with the data from Hopfinger and Toly (22). Both these numbers are lower than the value of 1.0 which has been widely used (9,11-19). The value of $\sigma_k$ adopted in this study is the average of those three $\sigma_k$ values, i.e.,

$$\sigma_k = (1.0 + 0.87 + 0.74)/3 = 0.87 \quad (\text{III-29})$$

The reason for using the average is that investigators (9,11-19,23,24) reported that predictions using the $k$-$\varepsilon$ model with $\sigma_k = 1.0$ gave some deviation from the experimental outcomes and could not adequately reflect the turbulence behavior for some situations, especially in the wake region (25,26).

The standard $k$-$\varepsilon$ model has difficulty describing the turbulence phenomena in the region where viscous effects are significant, e.g. near the wall. Consequently, several authors have sought to devise a modified model which is valid throughout the fully developed turbulent, transition, and laminar regions. An example is one proposed by Jones and Launder (23,24) who extended the standard $k$-$\varepsilon$ model to low-Reynolds-number flows by including the viscous diffusion of $k$ and $\varepsilon$ and by expressing some
coefficients in terms of the Reynolds number of turbulence. Their modified turbulence energy equation and its dissipation rate equation can be written to satisfy the whole flow region as follows:

\[
\rho \left( \frac{1}{r} \frac{\partial}{\partial r} (r \cdot V_k) + \frac{\partial}{\partial z} (\cdot V_k) \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( \cdot \frac{\nu_{eff}}{\sigma_k} \frac{\partial k}{\partial r} \right) + \frac{\partial}{\partial z} \left( \cdot \frac{\nu_{eff}}{\sigma_k} \frac{\partial k}{\partial z} \right) + C_1 \sigma - D_k \quad (III-30)
\]

\[
\rho \left( \frac{1}{r} \frac{\partial}{\partial r} (r \cdot V_\varepsilon) + \frac{\partial}{\partial z} (U_\varepsilon) \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( \cdot \frac{\nu_{eff}}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial r} \right) + \frac{\partial}{\partial z} \left( \cdot \frac{\nu_{eff}}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial z} \right) + C_1 \sigma - C_2 \rho \varepsilon \\
+ D_\varepsilon \quad (III-31)
\]

where \(D_k\) and \(D_\varepsilon\) represent the viscous diffusion of the turbulence energy and dissipation rate, respectively, and their mathematical expressions can be found in references (23, 24).

Launder and Spalding(9) recommend the following coefficients to be used with equations (III-30) and (III-31).

\[
\begin{align*}
C_\mu &= 0.09 \exp \left[ -2.5/\left(1+R_t/50\right) \right] \\
C_1 &= 1.44 \\
C_2 &= 1.92 \left[ 1.0 - 0.3 \exp(-R_t^2) \right]
\end{align*}
\]

where the turbulent Reynolds number \(R_t\) is defined by:

\[
R_t = \frac{\rho k^2}{\mu \varepsilon} \quad (III-33)
\]

The coefficient \(C_\mu\) was modified by Launder and Sharma(27) by including information from free shear flows to the following form:

\[
C_\mu = 0.09 \exp \left[ -3.4/\left(1+R_t/50\right)^2 \right]
\]

Unfortunately, the introduction of additional terms, \(D_k\) and \(D_\varepsilon\), in the transport equations of \(k\) and \(\varepsilon\) led to more computational time. Consequently, Lam and Bremhorst(28) did not use \(D_k\) and \(D_\varepsilon\) in equations
(III-31) and (III-32), but they re-expressed coefficients $C_1$, $C_2$ and $C_\mu$ as functions of the turbulent Reynolds number to account for the viscous effects. They used the following equations:

$$C_\mu = 0.09 (1 + 20.5/R_k^t) [1 - \exp(-0.0165R_k^t)]^2$$  \hspace{1cm} (III-34)

$$C_1 = 1.44 \left[1 + \frac{0.05}{(C_\mu/0.09)} \right]^3$$  \hspace{1cm} (III-35)

$$C_2 = 1.92 \left[1.0 - \exp(-R_k^t)\right]$$  \hspace{1cm} (III-36)

where $R_k^t$ is another turbulent Reynolds number which is given by:

$$R_k^t = \frac{\rho k^2 c_{yw}}{\mu}$$  \hspace{1cm} (III-37)

in which $y_w$ is the distance from the wall.

The aforementioned modified $k$-$\varepsilon$ model is unsuitable for swirling flows (9, 12, 12, 29), and further modification is desirable. In swirling flow the mean velocity has a rotational component. By adding one more term, $(\varepsilon/k)C_2 C_{Re} \cdot \varepsilon$, to the right hand side of equation (III-23) for $\varepsilon$, Launder, et al. (30) and Sharma (31) added the rotational effect on turbulence to the $k$-$\varepsilon$ model. The resulting equation for $\varepsilon$ is:

$$\rho \left[ \frac{1}{\rho} \frac{\partial}{\partial z} (\rho \varepsilon) + \frac{\partial}{\partial z} (\rho \varepsilon) \right] = \frac{1}{\rho} \frac{\partial}{\partial z} \left( \frac{\mu_{eff}}{\mu} \frac{\partial \varepsilon}{\partial z} \right) + \frac{\partial}{\partial z} \left( \frac{\mu_{eff}}{\mu} \frac{\partial \varepsilon}{\partial z} \right)$$

$$+ \frac{C_1 G - C_2 (1 - C_2 R_l \varepsilon)}{k}$$  \hspace{1cm} (III-38)

where the turbulent Richardson number, used by Launder, et al. (30) to account for the effects of the curvature and rotation, is defined by:

$$R_l = \frac{k^2 W}{\varepsilon^2} \frac{\partial (rW)}{\partial r}$$  \hspace{1cm} (III-39)
According to Launder, et al. (30), the coefficient $C_c$ was found to vary from zero to 0.5, and the optimum value was reported to be:

$$C_c = 0.2$$

We see in equation (III-39) that $R_i^t$ is negative when the angular momentum of the mean flow decreases with radius, and the new term in equation (III-38) will decrease the energy dissipation rate and will thus increase the turbulence kinetic energy. Also, the turbulent viscosity will become larger according to equation (III-25). Likewise, a positive value of $R_i^t$ will diminish the turbulent viscosity. As a result, swirling effect on the turbulence is incorporated in the term with the turbulent Richardson number in the $\varepsilon$-equation, and this causes a change in the turbulent viscosity. When the turbulent Richardson number is equal to zero, equation (III-38) reduces to equation (III-23).

The modified isotropic $k-\varepsilon$ model for swirling flows, composed of equations (III-22) and (III-38) where variables and coefficients are expressed in equations (III-19, 24, 25, 27, 29, 33-37, 39, 40), will be used as one of the turbulence models in this work. In this modified model, an isotropic eddy viscosity is still assumed, and the modification is accomplished by considering the swirling effects.

However, the isotropic $k-\varepsilon$ model discussed above will not be satisfactory when applied to two-dimensional axisymmetric flow in agitated vessels, because the important baffling effects are not included. The baffles convert the tangential flow to the axial and radial flow pattern as pointed out in Chapter I. To account for the baffling effects, Harvey and Greaves (6, Chapter II) added a drag term in the momentum equation for the angular velocity $W$. The drag term, $-C_{Dp}W^2/r$, was applied to the entire region of the tank. Based on their idea, a more elaborate drag
The angular momentum equation (III-17) becomes:
\[ \rho \frac{1}{r} \frac{\partial}{\partial r} (r \nu \frac{\partial \tau r}{\partial r}) + \frac{\partial}{\partial z} (\nu \frac{\partial \tau z}{\partial z}) + \rho \frac{1}{r} \frac{\partial}{\partial r} (r \nu \frac{\partial \tau r}{\partial r}) - \frac{2}{r} \frac{\partial}{\partial r} (\nu \partial r_x) + D_r \]  

(III-41)

where \( D_r \), the drag term to account for the baffling effects, is given by

\[ D_r = -C_{Drj} \frac{N_p W^2}{r} \] in jet zone  (III-42a)

\[ D_r = -C_{Drb} \frac{\rho (rW)^2}{ND_i^2 y_w (rx_w)^2} \] in bulk region  (III-42b)

where \( y_w \) is the distance from the tank wall, \( x_w \) is the distance from the tank bottom or liquid surface depending on the location of interest being in the lower or upper half of the tank, and \( N \) is the impeller speed. The two drag coefficients, \( C_{Drj} \) and \( C_{Drb} \), are two constants which need to be determined experimentally. The impeller speed and diameter are included in the drag terms because the flow in agitated vessels is created by rotating impellers. Different sizes and speeds of the impeller should have different drags caused by baffles. The closer to the tank wall the bigger the drag on the tangential flow becomes, and thus \( y_w \) is placed in the denominator of equation (III-42b). For the similar reason, \( x_w \) also appears in the denominator.

The jet zone for equation (III-42a) is defined as:

\[ x_w \geq \frac{1}{2}(H_i - H_b) \]  (III-43a)

where \( H_i \) is the height of the fluid in the tank, and \( H_b \) is the width of the blades of the impeller. The remaining region in the tank is the bulk or recirculation region, i.e.,
Using the continuity equation (III-12), the radial and axial momentum equations (III-16,18), the angular momentum equation (III-41) which accounts for the baffling effects, and the modified k-ε model for rotational flow, i.e., equation (III-22,38), we have a closed set of governing equations for the turbulent flow in the impeller-driven baffled reactor tanks. In this two-dimensional isotropic model, the assumption of the isotropic viscosity is applied to the entire region of the tank.

3.3.2 Nonisotropic Model

In the nonisotropic turbulence model, the viscosity may have six different components corresponding to the six Reynolds stresses. With this nonisotropic concept of the exchange coefficients (5-8,32-36), the equations of motion for the two-dimensional axisymmetric flow are written in the following form:

\[
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (r V^2) + \frac{\partial}{\partial z} (U^2) \right] = \frac{1}{r} \frac{\partial}{\partial r} \left( \nu_{rr} \frac{\partial V}{\partial r} \right) + \frac{\partial}{\partial z} \left( \nu_{rz} \frac{\partial V}{\partial z} \right) - \frac{\partial P}{\partial r} + \frac{V^2}{r^2}
\]

\[
- 2 \nu_{\theta \theta} \frac{V}{r^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( \rho \nu_{rr} \frac{\partial V}{\partial r} \right) + \frac{\partial}{\partial z} \left( \rho \nu_{rz} \frac{\partial U}{\partial r} \right)
\] (III-44)

\[
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (r U V) + \frac{\partial}{\partial z} (U W) \right] = \frac{1}{r} \frac{\partial}{\partial r} \left( \rho \nu_{rr} \frac{\partial U}{\partial r} \right) + \frac{\partial}{\partial r} \left( \rho \nu_{rz} \frac{\partial W}{\partial r} \right) - \frac{\partial P}{\partial r} + 2 \frac{\partial}{\partial r} \left( \rho \nu_{\theta \theta} \right)
\] (III-45)

\[
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (r U^2) + \frac{\partial}{\partial z} (U^2) \right] = \frac{1}{r} \frac{\partial}{\partial r} \left( \rho \nu_{rr} \frac{\partial U}{\partial r} \right) + \frac{\partial}{\partial r} \left( \rho \nu_{zz} \frac{\partial U}{\partial r} \right) - \frac{\partial P}{\partial r} + \rho g_z
\]

\[
+ \frac{1}{r} \frac{\partial}{\partial r} \left( \rho \nu_{rr} \frac{\partial U}{\partial r} \right) + \frac{\partial}{\partial z} \left( \rho \nu_{zz} \frac{\partial U}{\partial z} \right)
\] (III-46)

The k-ε model becomes:

\[
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (r \nu_k) + \frac{\partial}{\partial z} (U \nu_k) \right] = \frac{1}{r} \frac{\partial}{\partial r} \left( \nu_{rr} \frac{\partial k}{\partial r} \right) + \frac{\partial}{\partial z} \left( \nu_{zz} \frac{\partial k}{\partial z} \right) + C_{\text{non}} - \rho e
\] (III-47)
where the generation term in the nonisotropic k-ε model is given by:

\[ G_{\text{non}} = 2\left(\nu_{rr}\left(\frac{\partial v}{\partial r}\right)^2 + \nu_{\theta\theta}\left(\frac{\partial v}{\partial \theta}\right)^2 + \nu_{zz}\left(\frac{\partial v}{\partial z}\right)^2 + \nu_{\theta z}\left(\frac{2(\partial v)}{\partial \theta}\right)^2 + \nu_{e\theta}\left(\frac{2(\partial v)}{\partial \theta}\right)^2 + \nu_{e z}\left(\frac{2(\partial v)}{\partial z}\right)^2\right) \]

The model coefficients such as \( \sigma_k \) and \( C_1 \) in equations (III-47) and (III-48) are the same as those of isotropic k-ε model. When the six components of the viscosity are equal, the nonisotropic turbulence model reduces to the isotropic turbulence model.

Lilley, et al. (5-8,34) and Schetz (35) suggested using one of the six components as the effective viscosity, e.g. \( \nu_{rz} \). The effective viscosity \( \nu_{rz} \) in this nonisotropic model is the same as \( \nu_{\text{eff}} \) in the isotropic model, i.e.,

\[ \nu_{rz} = \nu + C_\mu \rho k^2/\varepsilon \]  

(III-50)

Then other viscosity components are obtained by using equation (III-50) and the so-called viscosity ratios, \( \sigma_{ij} \), which appear in the denominator of the right hand side in the following equations:

\[ \nu_{r\theta} = \frac{\nu_{rz}}{\sigma_{r\theta}} \]
\[ \nu_{\theta z} = \frac{\nu_{rz}}{\sigma_{\theta z}} \]
\[ \nu_{rr} = \frac{\nu_{rz}}{\sigma_{rr}} \]
\[ \nu_{\theta\theta} = \frac{\nu_{rz}}{\sigma_{\theta\theta}} \]
\[ \nu_{zz} = \frac{\nu_{rz}}{\sigma_{zz}} \]  

(III-51)
The values for these viscosity ratios are flow-dependent. Lilley, et al. (5-8,34) studied the free swirling jet and expressed the viscosity ratios as function of the local swirling number. The idea of the local swirling number of a free swirling jet is applied to our nonisotropic model, and we may express the viscosity ratios as:

$$\sigma_{ij} = a_{ij} + b_{ij} S_r^{1/3}$$  \hspace{1cm} (III-52)

where $a_{ij}$ and $b_{ij}$ are coefficients; and $S_r$, the local swirling number for the tangential jet from impeller, is defined by:

$$S_r = (10/D_i)(G_0/G_r)(D_i/r)^3$$  \hspace{1cm} (III-53)

In the above equation, $G_r$ is the constant radial flux of radial momentum, $G_0$ is the radial flux of angular momentum, and $D_i$ is the diameter of the impeller. $G_r$ and $G_0$ are defined by:

$$G_r = \int_{jet} \rho V^2 rdz$$  \hspace{1cm} (III-54)

$$G_0 = \int_{jet} \rho V\omega^2 dz$$  \hspace{1cm} (III-55)

where integral limit "jet" means the integrals are performed for the jet zone, defined by equation (III-43a).

In this study, the following values for the viscosity ratios are used in the jet zone:

$$\sigma_{r0} = 1 + 2S_r^{1/3}$$  \hspace{1cm} (III-56)

$$\sigma_{0z} = \sigma_{rr} = \sigma_{00} = \sigma_{zz} = 0.7$$  \hspace{1cm} (III-57)

The number 0.7 in the above equation was recommended by Lilley(34) for the free swirling jet and is adopted here for the tangential jet.
In the bulk region, which is defined by equation (III-43b), the viscosity ratios are given by:

\[
\sigma_{r\theta} = \sigma_{\theta z} = \sigma_{rr} = \sigma_{\theta \theta} = \sigma_{zz} = 1.0
\]  

(III-58)

The above equation means that the isotropic viscosity is assumed for the turbulent flow in the recirculation region of agitated vessels.

Using the closed set of equations (III-12,44-48), we can describe the turbulent flow in the stirred tanks without the isotropic assumption for the turbulent viscosity. The variables and coefficients in this nonisotropic model are given by equations (III-25,27,29,33-37,39,40, 49-51,53-58). In this nonisotropic model we do not need the drag term in the angular momentum equation to account for the baffling effects. This is because the vertical flow converted from the rotating flow by the baffles can be viewed as the extension of the jet stream pumped from the impeller. Thus, both swirling and baffling effects are considered in the nonisotropic k-\(\varepsilon\) model through different components of the viscosity in the jet zone.

3.4 General Form of the Governing Equations

In the previous sections, we have developed the conservation equations for the two-dimensional axisymmetrical flow in an agitated vessel. These include the continuity equation, momentum equations, and turbulence closure equations. They can be put in a general form as:

\[
\rho \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \sigma \nu \phi \right) + \frac{\partial}{\partial z} (\sigma \nu \phi) \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \tau _r \frac{\partial \phi}{\partial r} \right) + \frac{\partial}{\partial z} \left( \tau _z \frac{\partial \phi}{\partial z} \right) + S
\]

(III-59)

where \(\phi\) represents the dependent variable or property, \(\Gamma_{\phi}\) is the effective viscosity or diffusive transport coefficient corresponding to the
dependent variable, and \( S_\phi \) is the source term for the generation of the property associated with the dependent variable. The values for \( \phi \), \( \Gamma_\phi \) and \( S_\phi \) are listed in Table III-1 for the modified isotropic model and in Table III-2 for the nonisotropic model. The boundary conditions for these equations are given in the next section, and then we will embark on the formulation of the discretization equation of the general equation (III-59) to obtain the numerical solution.

3.5 Boundary Conditions for the Transport Equations

There are three kinds of boundary conditions. The first kind, also called Dirichlet-type, specifies values of variables on the boundary. The second kind, Neumann-type, specifies the flux of variables. The third kind or Robin-type are mixed boundary conditions of the first two kinds where an equation relates the value of the variable and its flux (or gradient) on the boundary.

For the agitated vessel with a centrally located impeller, the boundary conditions of the governing equations for the fluid dynamics are either Dirichlet or Neumann type. In Figure III-1 these boundary conditions are shown on a diagram for the flow in the vessel.

At the top of the liquid, the shear stress between the air and liquid is sufficiently small to have the velocity gradients with respect to \( z \) be zero. Also, the other \( z \)-direction gradients, i.e., \( k \) and \( \varepsilon \) are assumed zero. In addition, the axial velocity is zero since there is no flow across the interface.

At the faces of stationary solids, such as the tank wall, tank bottom, and baffles, the no slip conditions apply. Thus, three velocity components are equal to zero there. Also, velocity fluctuations must
Table III-1. Two-Dimensional Axisymmetric Governing Equations with the Isotropic Model.

<table>
<thead>
<tr>
<th>Conservation of</th>
<th>( \phi )</th>
<th>( \Gamma_\phi )</th>
<th>( S_\phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Axial momentum</td>
<td>( U )</td>
<td>( \mu_{\text{eff}} )</td>
<td>(- \frac{\partial P}{\partial z} + \rho g_z ) + ( \frac{1}{r} \frac{\partial}{\partial r} \left( r u_{\text{eff}} \frac{\partial U}{\partial z} \right) + \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial U}{\partial z}) )</td>
</tr>
<tr>
<td>Radial momentum</td>
<td>( V )</td>
<td>( \mu_{\text{eff}} )</td>
<td>(- \frac{\partial P}{\partial z} + \rho \frac{\partial V^2}{\partial z} - 2 \mu_{\text{eff}} \frac{V}{r} ) + ( \frac{1}{r} \frac{\partial}{\partial r} \left( r u_{\text{eff}} \frac{\partial V}{\partial z} \right) + \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial V}{\partial z}) )</td>
</tr>
<tr>
<td>Angular momentum</td>
<td>( rW )</td>
<td>( \mu_{\text{eff}} )</td>
<td>(- \frac{2}{r} \frac{\partial}{\partial r} (\mu_{\text{eff}} \frac{\partial W}{\partial r}) + D_r )</td>
</tr>
<tr>
<td>Turbulence kinetic energy</td>
<td>( k )</td>
<td>( \mu_{\text{eff}}/\sigma_k )</td>
<td>( G - \rho \varepsilon )</td>
</tr>
<tr>
<td>Energy dissipation rate</td>
<td>( \varepsilon )</td>
<td>( \mu_{\text{eff}}/\sigma_\varepsilon )</td>
<td>( \frac{1}{k} (C_1 G - C_2 (1 - C_3 R_L) \rho \varepsilon) )</td>
</tr>
</tbody>
</table>

where \( G = \nu (2(\frac{\partial V}{\partial r})^2 + \frac{V}{r})^2 + (\frac{\partial U}{\partial z})^2 + (\frac{\partial (U/r)}{\partial r})^2 + (\frac{\partial W}{\partial r})^2 + (\frac{\partial U}{\partial r})^2 + (\frac{\partial V}{\partial z})^2 \)  
\( D_r = -C_{Dr,j} N \rho w^2 \) in jet zone  
\( D_r = -C_{Dr,b} \rho (rw)^{1/2} / [N D_i^2 \gamma_w (rw)^{1/2}] \) in bulk region
### Table III-2. Two-Dimensional Axisymmetric Governing Equations with the Nonisotropic Model.

<table>
<thead>
<tr>
<th>Conservation of</th>
<th>$\phi$</th>
<th>$\Gamma_\phi$</th>
<th>$S_\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Axial momentum</td>
<td>$U$</td>
<td>$\mu_{rz}$</td>
<td>$-\frac{\partial p}{\partial z} + \rho g_z$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$+ \frac{1}{r} \frac{\partial}{\partial r}(r\nu_{rz} \frac{\partial V}{\partial z}) + \frac{\partial}{\partial z}(\mu_{zz} \frac{\partial U}{\partial z})$</td>
</tr>
<tr>
<td>Radial momentum</td>
<td>$V$</td>
<td>$\mu_{rz}$</td>
<td>$-\frac{\partial p}{\partial r} + \rho \frac{V^2}{r} - 2\nu_{\theta \theta} \frac{V}{r}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$+ \frac{1}{r} \frac{\partial}{\partial r}(r\nu_{rr} \frac{\partial V}{\partial r}) + \frac{\partial}{\partial r}(\mu_{rr} \frac{\partial U}{\partial r})$</td>
</tr>
<tr>
<td>Angular momentum</td>
<td>$rW$</td>
<td>$\mu_{rz}$</td>
<td>$-\frac{2}{r} \frac{\partial}{\partial z}(\nu_{xz} rW)$</td>
</tr>
<tr>
<td>Turbulence kinetic energy</td>
<td>$k$</td>
<td>$\mu_{rz}/\sigma_k$</td>
<td>$\frac{\epsilon}{\sigma_k} (G_{non} - \rho \epsilon)$</td>
</tr>
<tr>
<td>Energy dissipation rate</td>
<td>$\epsilon$</td>
<td>$\mu_{rz}/\sigma_\epsilon$</td>
<td>$\frac{\epsilon}{k} (C_1 G_{non} - C_2 (1 - C_c R_l) \rho \epsilon)$</td>
</tr>
</tbody>
</table>

where $G_{non} = 2(\nu_{xx} \frac{\partial V}{\partial z})^2 + \nu_{\theta \theta} \frac{V}{r} \frac{\partial V}{\partial z} + \nu_{zz} \frac{\partial U}{\partial z}^2 + \nu_{\theta \theta} (\frac{\partial (W/r)}{\partial z})^2 + \nu_{zz} (\frac{\partial W}{\partial z})^2 + \nu_{xz} (\frac{\partial W}{\partial z})^2$.
Figure III-1. Boundary conditions for flow in an agitated vessel.

\[
\frac{\partial \phi}{\partial z} = 0 \quad \text{except} \quad U = 0
\]

\[
\frac{\partial \phi}{\partial r} = 0 \quad \text{except} \quad U = 0, \quad V = 0, \quad W = \pi r N.
\]

\[
\frac{\partial \phi}{\partial r} = 0 \quad \text{except} \quad U, V, W \text{ from tangential jet model}
\]
vanish at stationary rigid surfaces, and both \( k \) and \( \varepsilon \) are equal to zero there. These boundary conditions also apply for the interior of the rotating solids, such as the shaft of the impeller.

At the surface of the shaft, the axial and radial velocities are zero while the angular velocity is assumed to be the surface velocity of the shaft. There is no flux across the shaft, and the gradients of other variables are zero. At the centerline of the tank, the radial and angular velocity components are zero. Besides, all \( r \)-direction gradients are zero because of symmetry along the centerline of the tank.

As discussed in Chapter II, the impeller region is accurately described as a tangential jet. The equations for the velocity components in the jet stream, i.e., equations (11-6,7,8), are used as boundary conditions at the impeller tip. As for the other variables such as \( k \) and \( \varepsilon \), their gradients with respect to \( r \) at the blade tip are taken as zero for the boundary conditions there.

For the top and bottom faces of the rotating blades, the gradients with respect to \( z \) of all variables except axial and tangential velocity components are assumed to be zero. The boundary conditions of axial velocity there is obtained from the material balance over the blade-swept region, which is performed in Appendix A. The tangential velocity in this region is obtained based on the assumption of the solid rotation for the impeller. Expressions for both velocity components will be presented in Section 3.9 Boundary Conditions in Numerical Representations.

3.6 Two-Dimensional Finite Domain Formulation

The general differential equations (III-59) for the fluid dynamics in agitated vessels has been derived. In this section the numerical solution
of these equations will be described. There are a number of methods for the numerical solution procedure, and the most famous one may be the Taylor-series formulation of finite-difference equations. Unfortunately, this method of formulation is difficult to apply in the three-dimensional cylindrical coordinate system when variable spacing is highly desirable. The variational formulation is another method which is widely employed in finite-element methods for the problems of stress analysis. However, a variational principle for the steady-state Navier-Stokes equations does not exist according to Finlayson \(37\) which eliminates the variational formulation. The finite domain method, which is easy and flexible to be applied in both two- and three-dimensional partial differential equations, is adopted here to develop the discretization equations for the numerical solution. In this method, the whole calculation domain is divided into finite subdomains, and the differential equations are integrated over each of them. Thus, integral equations are obtained for all finite domains or control volumes. Profiles (or basis functions in the finite-element jargon) express how a property \(\phi\) varies between the grid points and are used to evaluate the integrals. This leads to the discretized form of the general differential equations.

3.6.1 General Derivation

Proceeding as described above to obtain the discretization equation, equation (III-59) is multiplied by \(r\) and integrated with respect to \(r\) and \(z\) over the finite domain which includes \(w\) to \(e\) on \(r\) and \(b\) to \(t\) on \(z\) as shown in Figure III-2. The result is given below.
Figure III-2. Locations of the grid points and control faces in a finite domain scheme.
$$\rho \left( \frac{\partial}{\partial z} (rV_e) \right) dz + \rho \left( \frac{\partial}{\partial z} (U_0) \right) dz = \int_b \int_c \frac{\partial}{\partial z} (r_{\phi} \frac{\partial}{\partial z}) drdz$$

$$+ \int_b \int_c \frac{\partial}{\partial z} (r_{\phi} \frac{\partial}{\partial z}) drdz + \int_b \int_c \frac{\partial}{\partial z} S_z dzdr$$

(III-60)

The symbols w, e, b, and t represent the surfaces of the finite domain on the west, east, bottom, and top sides, respectively. The locations of these control surfaces and grid points are shown in Figure III-2, where symbol P stands for the grid point being considered, and capitals W, E, B, and T represent the four neighboring grid points in the radial and axial direction. All grid points are located at the geometrical centers of the subdomain, but the control volume dimensions or subdomains are not necessarily uniform. The spacings corresponding to the finite domain scheme can vary and are given in Figure III-3. The use of non-uniform grid scheme is desirable for those regions close to the impeller, tank wall and baffles where more grid points are needed since gradients in the flow are larger in these regions.

Assuming a piecewise linear profile equation (III-60) can be integrated to give:

$$\rho \left[ (rV_e - (rV_w) \right] \Delta z + \rho \left[ (U_0) - (U_b) \right] \left( \frac{r_e + r_w}{2} \right) \Delta z =$$

$$\left[ \left( r_{\phi} \frac{\partial}{\partial z} e \right) - \left( r_{\phi} \frac{\partial}{\partial z} w \right) \right] \Delta z + \left[ \left( r_{\phi} \frac{\partial}{\partial z} e \right) - \left( r_{\phi} \frac{\partial}{\partial z} b \right) \right] \left( \frac{r_e + r_w}{2} \right) \Delta z$$

$$+ S_z \left( \frac{r_e + r_w}{2} \right) \Delta r \Delta z$$

(III-61)

and rearranging the above equation gives

$$\left( \rho (rV) e - (rV) w \right] \Delta z + \rho (U_0) - (U_b) \left( \frac{r_e + r_w}{2} \right) \Delta z$$

$$\left[ \left( r_{\phi} \frac{\partial}{\partial z} e \right) - \left( r_{\phi} \frac{\partial}{\partial z} w \right) \right] \Delta z + \left[ \left( r_{\phi} \frac{\partial}{\partial z} e \right) - \left( r_{\phi} \frac{\partial}{\partial z} b \right) \right] \left( \frac{r_e + r_w}{2} \right) \Delta z$$

$$- S_z \left( \frac{r_e + r_w}{2} \right) \Delta r \Delta z = 0$$

(III-62)
Figure III-3  Spacings corresponding to the finite domain scheme in Figure III-2.
Those equations are non-linear and coupled. Thus, an iteration scheme is necessary, and this will require an initial estimate of the dependent variables and a procedure to iteratively move to a converged solution of equation (III-62). This procedure will consider that the velocity components and source term are known, and that \( \phi \) is the only variable in equation (III-62). The task is to relate \( \phi \) and the partial derivatives of \( \phi \) on control surfaces to \( \phi \) at the grid points such that the discretized form can be achieved. In other words, the expressions in the two braces in equation (III-62) should be substituted by the following equations:

\[
\begin{align*}
 [\rho U T e - (r_{\phi} \frac{\partial \phi}{\partial z}_e)] - [\rho u_b \phi_b - (r_{\phi} \frac{\partial \phi}{\partial z}_b)] = \\
 [\rho U T e p + A_T(\phi_p - \phi_T)] - [\rho u_b \phi_p + A_B(\phi_B - \phi_p)] \\
 (III-63)
\end{align*}
\]

\[
\begin{align*}
 [\rho(r V)e \phi_e - (r r_{\phi} \frac{\partial \phi}{\partial z})_e] - [\rho(r V)w \phi_w - (r r_{\phi} \frac{\partial \phi}{\partial z})_w] = \\
 [\rho r w \phi_p + A_w(\phi_w - \phi_p)] - [\rho r w \phi_p + A_w(\phi_w - \phi_p)] \\
 (III-64)
\end{align*}
\]

After the substitution, equation (III-62) become:

\[
\begin{align*}
 [\rho r w e - \rho r w w \Delta z] + (\rho U_T - \rho U_b)(\frac{r e + r w}{2} \Delta T) & + [A_E(\phi_p - \phi_E) \\
 - A_W(\phi_w - \phi_p) \Delta z] + [A_T(\phi_p - \phi_T) - A_B(\phi_B - \phi_p)](\frac{r e + r w}{2} \Delta T) \\
 - S_T\left(\frac{r e + r w}{2}\right) \Delta r \Delta z = 0 \\
 (III-65)
\end{align*}
\]

In this equation all \( \phi \)'s are at the grid points, and the coefficients \( A_T, A_B, A_E, \) and \( A_W \) needs to be determined.

The central difference and upwind scheme were the two common methods developed for this purpose. However, they have stability and accuracy problems for the solution of convection-diffusion problems. The hybrid scheme, developed by Spalding(38), combined the better features of the two
previous ones. It is the same as the central difference scheme for Peclet numbers, the ratio of convective transport to diffusive flux, in the range $-2 \leq N_p \leq 2$ where the diffusion effect is dominant; and outside this range where convection is dominant it is the upwind scheme. Because the hybrid scheme can be used to solve both high- and low-Reynolds-number problems, it is widely applied to numerical transport studies.

However, the exponential scheme proposed and employed by Raithy and Torrance(39) is superior to the hybrid scheme. It is based on the exponential solution of the one-dimensional convection-diffusion problems. This scheme is not widely used because exponentials are very expensive to compute, and it is not exact for two- and three-dimensional cases where sources exist. A good approximation to the exponential scheme is preferred, and the exponential scheme has become a criterion for comparison according to Patankar(40). It has been shown that the central difference scheme deviates widely from the exponential scheme when the Peclet number becomes large, the upwind scheme deviates when the Peclet number is small and the hybrid scheme is a good three-range approximation to the exponential scheme. The hybrid scheme has been said to give physically realistic solutions for relatively coarse grids(40). For a value of the Peclet number of ±2, the intersections between the three ranges, there is large deviation from the exponential scheme. To reduce the departure, Patankar(40) suggested using the power-law scheme, which is a four-range approximation to the exponential scheme. The power-law expression for $A_T$ in equation (III-65) can be written as:

$$A_T = -\rho U_t$$

for $N_{pt} < -10$  \hspace{1cm} (III-66a)

$$A_T = (\Gamma_{pt}/\delta z_t)(1+0.1N_{pt})^5 - \rho U_t$$

for $-10 \leq N_{pt} < 0$  \hspace{1cm} (III-66b)
\[ A_T = \left( \frac{\Gamma_{\phi t}}{\delta z_t} \right) (1-0.1N_{pt})^5 \]  
for \(0 \leq N_{pt} \leq 10\) (III-66c)

\[ A_T = 0 \]  
for \(10 < N_{pt}\) (III-66d)

Likewise, \(A_B\) in the power-law scheme can be expressed as:

\[ A_B = 0 \]  
for \(N_{pb} < -10\) (III-67a)

\[ A_B = \left( \frac{\Gamma_{\phi b}}{\delta z_b} \right) (1+0.1N_{pb})^5 \]  
for \(-10 \leq N_{pb} < 0\) (III-67b)

\[ A_B = \left( \frac{\Gamma_{\phi b}}{\delta z_b} \right) (1-0.1N_{pb})^5 + \rho U_b \]  
for \(0 \leq N_{pb} \leq 10\) (III-67c)

\[ A_B = \rho U_b \]  
for \(10 < N_{pb}\) (III-67d)

In equations (III-66) and (III-67) the Peclet numbers at the top face, \(N_{pt}\), and at the bottom face, \(N_{pb}\), are defined by:

\[ N_{pt} = \frac{\rho U_t}{\Gamma_{\phi t}/\delta z_t} \]  
(III-68a)

\[ N_{pb} = \frac{\rho U_b}{\Gamma_{\phi b}/\delta z_b} \]  
(III-68b)

where distances \(\delta z_t\) and \(\delta z_b\) are shown in Figure III-3.

Equations (III-66) and (III-67) can be rewritten in the following compact form:

\[ A_T = \left( \frac{\Gamma_{\phi t}}{\delta z_t} \right) [0,(1-0.1|N_{pt}|)^5]'_{\text{max}} + [0,-\rho U_t]'_{\text{max}} \]  
(III-69)

\[ A_B = \left( \frac{\Gamma_{\phi b}}{\delta z_b} \right) [0,(1-0.1|N_{pb}|)^5]'_{\text{max}} + [\rho U_b,0]'_{\text{max}} \]  
(III-70)

where the symbol \([x_1, x_2]'_{\text{max}}\) represents the greater of \(x_1\) and \(x_2\), and is equivalent to AMAX1(x(1),x(2)) in a FORTRAN program. Similarly, \(A_E\) in equation (III-65) are given by:

\[ A_E = \left( \frac{\Gamma_{\phi e}}{\delta r_e} \right) [0,(1-0.1|N_{pe}|)^5]'_{\text{max}} + [0,-\rho V_e]'_{\text{max}} \]  
(III-71)
\[ A_W = (\Gamma_{\phi W}/\delta r_w)[0,(1-0.1|N_{p w}|)^9]_{\text{max}} + [pV_w,0]_{\text{max}} \quad (III-72) \]

The Péclet numbers on the east- and west-side faces are defined as:

\[ N_{p e} = \rho V_e / (\Gamma_{\phi e}/\delta r_e) \quad (III-73a) \]

\[ N_{p w} = \rho V_w / (\Gamma_{\phi w}/\delta r_w) \quad (III-73b) \]

where spacings \( \delta r_e \) and \( \delta r_w \) are shown in Figure III-3.

The values of \( \Gamma_{\phi} \) are known only at the grid points, and those values of the \( \Gamma_{\phi} \)'s at the control surfaces in equations (III-68) to (III-70) and (III-71) to (III-73) have to be suitably expressed in terms of grid-point \( \Gamma_{\phi} \)'s. Referring Figure III-3 consider that the control volume surrounding the grid point \( P \) is composed of a material of uniform \( \Gamma_{\phi P} \), and the one around point \( E \) is composed of uniform \( \Gamma_{\phi E} \). Thus, from the balance of diffusive flux through this "composite slab" we can have

\[ \Gamma_{\phi e}e = \left[ \frac{r_e(1-f_e)}{r_P\Gamma_{\phi P}} + \frac{r_{eF}}{r_{PE}\Gamma_{\phi E}} \right]^{-1} \quad (III-74) \]

where \( f_e = \delta r_{e+}/\delta r_e \). Similarly in the \( z \)-direction, we have

\[ \Gamma_{\phi z} = \left[ \frac{1-f_z}{\Gamma_{\phi P} + \Gamma_{\phi T}} \right]^{-1} \quad (III-75) \]

where \( f_z = \delta z_{e+}/\delta z_e \). Likewise, we can have the similar expressions for \( \Gamma_{\phi W} \) and \( \Gamma_{\phi b} \).

Equation (III-65) can be put in a more convenient form using the continuity equation. If the continuity equation (III-12) is multiplied by \( r \), and integrated with respect to \( r \) and \( z \) over the control volume in Figure III-2, the discrete form of the continuity equation is as follows:

\( (III-76) \)
Using equation (III-76) to eliminate the expressions in the first bracket in equation (III-65) and rearranging gives the linear form of the discretization equation for \( \phi \) at the point \( P \) in terms of \( \phi \) at four neighboring points \( T, B, E, \) and \( W \).

\[
C_p \phi_P = C_T \phi_T + C_B \phi_B + C_E \phi_E + C_W \phi_W + C_S \phi
\]

(III-77)

where

\[
C_T = A_T \left( \frac{r_e + r_w}{2} \right) \Delta x
\]

(III-78a)

\[
C_B = A_B \left( \frac{r_e + r_w}{2} \right) \Delta x
\]

(III-78b)

\[
C_E = A_E r_e \Delta z
\]

(III-78c)

\[
C_W = A_W r_w \Delta z
\]

(III-78d)

\[
C_p = C_T + C_B + C_E + C_W
\]

(III-78e)

\[
C_S \phi = S \phi \left( \frac{r_e + r_w}{2} \right) \Delta x \Delta z
\]

(III-78f)

Equation (III-77) tells us how \( \phi_P \), the variable on the central grid point, is affected by its four neighboring \( \phi \)'s through the four corresponding coefficients which include the effects of diffusion and convection. These neighboring-point coefficients must have the same sign as the coefficient of the central grid point. The reason is a negative coefficient would cause a decrease in the property at \( P \) from an increase in the property at a neighboring point, which is physically impossible. The \( C_S \phi \) in equation (III-77) includes a source term \( S \phi \) as shown in equation (III-78f), and from Table III-1 and III-2 we see that it is often a non-linear function of the dependent variable \( \phi \) itself. Consequently, it is necessary to
linearize this term as follows to complete a set of linear algebraic equations.

\[ S_\phi = S_{\phi 1} + S_{\phi 2} \phi_p \quad (III-79) \]

After this linearization of the source term, equation (III-77) retains the same form. The coefficients associated with the neighboring points to the central point have no changes from equations (III-78 a-d), but the coefficients for the grid point and the source term have to be rewritten as follows:

\[ C_p = C_T + C_B + C_E + C_W - S_{\phi 2} \left( \frac{r_e + r_w}{2} \right) \Delta \tau \Delta z \quad (III-78g) \]

\[ C_{S\phi} = S_{\phi 1} \left( \frac{r_e + r_w}{2} \right) \Delta \tau \Delta z \quad (III-78h) \]

Note that \( S_{\phi 2} \) in equation (III-78g) must be negative such that all the coefficients for the grid points are of the same sign as we discussed previously.

The values of the velocity components in the axial and radial direction are needed for the iterative solution of equation (III-77). These velocities are located in the surfaces of finite domain about \( P \) as shown in Figure III-2. Thus, a staggered grid for the velocity components is used as shown in Figures III-4 and III-5 for \( U_t \) and \( V_e \), and this approach was first employed by Harlow and Welch(41) in their Marker-and-Cell Method and has become a very common construction. Simply replacing \( \phi \) with \( U_t \) in the general linear algebraic equation (III-77) and changing the subscripts associated with the staggered finite domain in Figure III-4, we can obtain the discretization equation for the \( z \)-component of the momentum equations as follows:
Figure III-4. Finite domain for the velocity in the z-direction.
Figure III-5. Finite domain for the velocity in the r-direction.
Similarly, the discretization equation for the radial momentum equation is given by:

\[ C_e V_e = \sum_{n} C_{n} V_{n} + C_{S} \frac{r_e + r_{e}^{+}}{2} \Delta r_e \] (III-81)

The symbol \( \sum \) represents the summation, and the subscript \( nb \) in these two equations stands for neighbors which are pointed out by arrows in Figures III-4 and III-5. For a two-dimensional problem the number of neighbor terms is four. All the coefficients in the above two equations have the same expressions to equations (III-78 a-d, g-h). Here the pressure terms have been separated from the source terms in equations (III-80) and (III-81). In the subsequent section, this procedure will be applied to obtain the discretized angular momentum equation in the three-dimensional flowfield. In two-dimensional cases, general discretization equation (III-77) can be applied without changing subscripts since no staggered grid for angular velocity is needed for two-dimensional axisymmetric flow.

The discretized momentum equations (III-80) and (III-81) require a known pressure field. The pressure field is one of the variables and must be estimated for the solution of velocity field. The discretized continuity equation (III-76) is used as a convergence criterion to have the correct velocity field be generated with equations (III-80) and (III-81). In two-dimensional cases the pressure field can be eliminated by cross-differentiating the radial and axial momentum equations. This method is known as stream function and vorticity transformations and is only applicable to two-dimensional flows. However the turbulent flow in a mechanically agitated vessel is three-dimensional, we then have to use a
method which converges the pressure field along with the velocity field\((40,42)\). This is discussed in the next subsection.

3.6.2 The Pressure Equation:

To derive an equation representing the pressure field, we start with the momentum equation in the form of equations (III—80) and (III—81). These equations can be rewritten as follows:

\[
U_t = \frac{1}{C_e} \{ \Sigma C_{nb} V_{nb} + C_{S_f} \} + \frac{1}{C_e} (P_P - P_T)(\frac{r_e + r_T}{2} \Delta r)_t
\]

(III—82)

\[
V_e = \frac{1}{C_e} \{ \Sigma C_{nb} V_{nb} + C_{S_f} \} + \frac{1}{C_e} (P_P - P_E)(r_e \Delta z)_e
\]

(III—83)

For simplicity, let the first term on the right hand side in the above two equations be represented by \(\hat{U}_t\) and \(\hat{V}_e\), i.e.,

\[
\hat{U}_t = \frac{1}{C_e} \{ \Sigma C_{nb} V_{nb} + C_{S_f} \}
\]

(III—84)

\[
\hat{V}_e = \frac{1}{C_e} \{ \Sigma C_{nb} V_{nb} + C_{S_f} \}
\]

(III—85)

Then the equations (III—82) and (III—83) can be written as:

\[
U_t = \hat{U}_t + \frac{1}{C_e} (P_P - P_T)(\frac{r_e + r_T}{2} \Delta r)_t
\]

(III—86)

\[
V_e = \hat{V}_e + \frac{1}{C_e} (P_P - P_E)(r_e \Delta z)_e
\]

(III—87)

Similarly, the other two velocities \(U_b\) and \(V_w\) are given by:
These four velocity components must satisfy the continuity equation. The discretized form of the continuity equation, i.e., equation (III-76), contains these components. Using the above equations to eliminate these components in equation (III-76), the result is one in terms of the pressure only as given below.

\[
 CpPp = C_T P_T + C_B P_B + C_E P_E + C_W P_W + C_S
\]

where the coefficients are:

\[
 C_T = \rho \frac{1}{C_e} \left( \frac{r_e^2 + r_w^2}{2} \Delta x \right)_e \left( \frac{r_e^2 + r_w^2}{2} \Delta x \right) \\
 C_B = \rho \frac{1}{C_b} \left( \frac{r_e^2 + r_w^2}{2} \Delta x \right)_b \left( \frac{r_e^2 + r_w^2}{2} \Delta x \right) \\
 C_E = \rho \frac{1}{C_e} (r_e \Delta z)_e (r_e \Delta z) \\
 C_W = \rho \frac{1}{C_w} (r_w \Delta z)_w (r_e \Delta z) \\
 C_P = C_T + C_B + C_E + C_W \\
 C_S = -\rho \left( \hat{U_e} - \hat{U_b} \right) \frac{r_e^2 + r_w^2}{2} \Delta x + \rho (r_e \hat{V_e} - r_w \hat{V_w}) \Delta z
\]

The pressure field calculated from equation (III-90) may be used as the estimated pressure field for the calculation of the velocity field. If the correct velocity field is finally obtained, the corresponding pressure
field is also correct since at that moment the continuity equation is satisfied.

3.6.3 Corrections of the Velocity Field:

A procedure to speed convergence can be developed which provides a correction to the velocity field rather than use the values from the previous iteration. First, the estimated pressure field is denoted $P^*$, and the resulting velocity field is represented by $U^*$ and $V^*$ which came from the solution of the discretized momentum equations, equations (III-80) and (III-81) as written below with a * superscript.

$$C_{L'}U_{t}^* = \Sigma C_{nb}U_{rb}^* + C_{S_f} + (P_{P}^* - P_{T}^*)\left(\frac{r_e + r_w}{2}\Delta r\right)_{t}$$ (III-80a)

$$C_{e}V_{e}^* = \Sigma C_{nb}V_{rb}^* + C_{S_f} + (P_{P}^* - P_{E}^*)(r_e\Delta z)_{e}$$ (III-81a)

To have an improved velocity field for the next iteration, Patankar and Spalding(42) proposed velocity and pressure corrections. Instead of solving the pressure equation (III-90) for pressure, they obtained the pressure field using the pressure correction $P'$ as follows:

$$P = P^* + P'$$ (III-92)

Patankar and Spalding(42) suggested using the following corrected velocity field for the next iteration.

$$U_{t} = U_{t}^* + \frac{1}{C_{t}}(P_{P}' - P_{T}')\left(\frac{r_e + r_w}{2}\Delta r\right)_{t}$$ (III-93)

$$V_{e} = V_{e}^* + \frac{1}{C_{e}}(P_{P}' - P_{E}')(r_e\Delta z)_{e}$$ (III-94)

$$U_{b} = U_{b}^* + \frac{1}{C_{b}}(P_{B}' - P_{P}')\left(\frac{r_e + r_w}{2}\Delta r\right)_{w}$$ (III-95)
The first term in the right hand side of the above four equations is the velocity field calculated from the discretized momentum equations. The second term is the velocity corrections to speed the convergence.

To obtain an equation for pressure corrections appearing in equations (III-92) to (III-96), Patankar and Spalding(42) suggested using the discretized continuity equation. Substituting equations (III-93) to (III-96) into equation (III-76), we may obtain a discretization equation for $P'$, i.e., the pressure-correction equation.

$$C_p P'_w = C_T P'_T + C_B P'_B + C_E P'_E + C_W P'_W + C_S$$

where $C_T$, $C_B$, $C_E$, $C_W$, and $C_p$ are given by equations (III-91 a-e), and $C_S$ is given by:

$$C_S = -[\rho(U_e - U_b) \frac{r_e + r_w}{2} \Delta r + \rho(r_e v_e - r_w v_w) \Delta z]$$

The right hand side of equation (III-98) is the same as the continuity equation (III-76). If $C_S$ in the pressure-correction equation is zero, the starred velocity field has satisfied the continuity equation, and a converged velocity field has been obtained. Also, the starred pressure field is the converged solution. If $C_S$ is not zero, the continuity equation has not been satisfied, and the starred pressure and velocity field have not converged. More iterations are then necessary until the source term of equation (III-97) becomes zero; i.e., the continuity equation has been satisfied.
3.7 Extensions for a Three-Dimensional Flow Field

In the previous sections the conservation laws were written for two-dimensional axisymmetrical flow for the convenience of having fewer terms in the development of the discretization equations. In this section, we will include those additional terms for the description of three-dimensional steady flow in an agitated vessel. The assumption of axisymmetry is only approximate, and it ignores the flow around the baffles. The tank baffles create property gradients in the tangential direction. The flow is three-dimensional, and this was shown in Mulvahill's measurements (6, Chapter I). It is necessary to show what extensions are required for the differential and discretized transport equations from two- to three-dimensional cases.

3.7.1 Conservation Equations in the Isotropic Model

In section 3.2, the continuity equation and momentum equations were presented for three-dimensional flow. Using the concepts developed for the two-dimensional isotropic model in which the isotropic eddy viscosity was assumed to represent the Reynolds stress terms, we may obtain the following general transport equations for the three-dimensional flow which is an extension of equation (III-59).

\[
\frac{1}{\rho} \frac{\partial}{\partial z} (\rho U^r) + \frac{1}{\rho} \frac{\partial (\rho U^r)}{\partial y} + \frac{\partial}{\partial z} (\rho U^r) = \frac{1}{\rho} \frac{\partial}{\partial z} \left( \frac{\partial \rho}{\partial z} \right) + \frac{\partial}{\partial z} \left( \frac{\partial \rho}{\partial z} \right) + S_r
\]  

Continuity equation \((\phi=1, \Gamma_\phi=0)\) is an extension of equation (III-12):

\[
\frac{1}{\rho} \frac{\partial (\rho V)}{\partial x} + \frac{1}{\rho} \frac{\partial (\rho W)}{\partial y} + \frac{\partial (\rho U)}{\partial z} = 0
\]  

(III-100)
Radial momentum equation ($\phi=V, \Gamma_\phi=\mu_{\text{eff}}$) is an extension of equation (III-16):

$$
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (rV) + \frac{1}{r} \frac{\partial}{\partial \theta} (\theta V) + \frac{\partial}{\partial z} (z V) \right] = \frac{1}{r} \frac{\partial}{\partial r} (r\mu_{\text{eff}} \frac{\partial V}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial \theta} (r\mu_{\text{eff}} \frac{\partial V}{\partial \theta})
+ \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial V}{\partial z}) - \frac{\partial P}{\partial r} + \frac{2}{r} \mu_{\text{eff}} \frac{V}{r^2} - 2 \frac{\mu_{\text{eff}}}{r^2} \frac{\partial V}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} (r\mu_{\text{eff}} \frac{\partial V}{\partial r})
+ \frac{1}{r} \frac{\partial}{\partial \theta} (r\mu_{\text{eff}} \frac{\partial (V/r)}{\partial r}) + \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial V}{\partial z}) 
$$

(III-101)

Angular momentum equation ($\phi=rW, \Gamma_\phi=\mu_{\text{eff}}$) is an extension of equation (III-17):

$$
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (rW^2) + \frac{1}{\theta} \frac{\partial}{\partial \theta} (\theta W) + \frac{\partial}{\partial z} (z W) \right] = \frac{1}{r} \frac{\partial}{\partial r} (r\mu_{\text{eff}} \frac{\partial W}{\partial r})
+ \frac{1}{\theta} \frac{\partial}{\partial \theta} (\mu_{\text{eff}} \frac{\partial W}{\partial \theta}) - \frac{\partial P}{\partial r} - 2 \frac{\mu_{\text{eff}}}{r} \frac{rW}{r^2} + \frac{1}{r} \frac{\partial}{\partial r} (r\mu_{\text{eff}} \frac{\partial W}{\partial r})
+ \frac{1}{\theta} \frac{\partial}{\partial \theta} (\mu_{\text{eff}} \frac{\partial W}{\partial \theta}) + 2 \frac{\mu_{\text{eff}}}{r} \frac{\partial W}{\partial r} + \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial W}{\partial z})
$$

(III-102)

Axial momentum equation ($\phi=U, \Gamma_\phi=\mu_{\text{eff}}$) is an extension of equation (III-18):

$$
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (rUV) + \frac{1}{\theta} \frac{\partial}{\partial \theta} (\theta UV) + \frac{\partial}{\partial z} (z UV) \right] = \frac{1}{r} \frac{\partial}{\partial r} (r\mu_{\text{eff}} \frac{\partial U}{\partial r}) + \frac{1}{\theta} \frac{\partial}{\partial \theta} (\mu_{\text{eff}} \frac{\partial U}{\partial \theta})
+ \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial U}{\partial z}) - \frac{\partial P}{\partial r} + \rho g + \frac{1}{r} \frac{\partial}{\partial r} (r\mu_{\text{eff}} \frac{\partial V}{\partial z}) + \frac{1}{r} \frac{\partial}{\partial r} (r\mu_{\text{eff}} \frac{\partial W}{\partial z})
+ \frac{\partial}{\partial z} (\mu_{\text{eff}} \frac{\partial U}{\partial z})
$$

(III-103)

Equation of turbulence kinetic energy ($\phi=k, \Gamma_\phi=\mu_{\text{eff}}/\sigma_k$) is an extension of equation (III-22):
\[
\rho \left[ \frac{1}{\partial \tau} (\tau V_k) + \frac{1}{\partial \zeta} (\tau U_k) + \frac{\partial}{\partial \zeta} (U_k) \right] = \frac{1}{\partial \tau} (\tau \frac{\partial v_{\text{eff}}}{\partial \kappa} \frac{\partial \kappa}{\partial \tau}) \\
+ \frac{1}{\partial \zeta} \left( \frac{1}{\partial \zeta} \frac{\partial v_{\text{eff}}}{\partial \kappa} \frac{\partial \kappa}{\partial \zeta} \right) + \frac{1}{\partial \zeta} \left( \frac{\partial v_{\text{eff}}}{\partial \kappa} \frac{\partial \kappa}{\partial \zeta} \right) + G - \rho \varepsilon
\]

(III-104)

Equation of energy dissipation rate \((\varphi = \varepsilon, \Gamma_{\varphi} = v_{\text{eff}} / \sigma_{\varepsilon})\) is an extension of equation (III-38):

\[
\rho \left[ \frac{1}{\partial \tau} (\tau V_e) + \frac{1}{\partial \zeta} (\tau U_e) + \frac{\partial}{\partial \zeta} (U_e) \right] = \frac{1}{\partial \tau} (\tau \frac{\partial v_{\text{eff}}}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial \tau}) \\
+ \frac{1}{\partial \zeta} \left( \frac{1}{\partial \zeta} \frac{\partial v_{\text{eff}}}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial \zeta} \right) + \frac{1}{\partial \zeta} \left( \frac{\partial v_{\text{eff}}}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial \zeta} \right) \\
+ \frac{\partial}{\partial \zeta} \frac{\partial v_{\text{eff}}}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial \zeta} + \frac{\varepsilon}{\kappa} \left[ C_1 G - C_2 (1 - C_3 R_k \rho \varepsilon) \right]
\]

(III-105)

The empirical constants and parameters of the above governing equations are given as follows:

\[ v_{\text{eff}} = \mu + \mu_t \]

(III-19)

\[ \mu_t = C_\mu \frac{\rho k^2}{\varepsilon} \]

(III-25)

\[ C_\mu = 0.09 \left[ 1 + 20.5 / R_k \right] \left[ 1 - \exp(-0.0165 R_k) \right]^2 \]

(III-34)

\[ C_1 = 1.44 \left[ 1 + (0.05 / (C_\mu / 0.09))^2 \right] \]

(III-35)

\[ C_2 = 1.92 \left[ 1.0 - \exp(-R_t^2) \right] \]

(III-36)

\[ R_t = \rho k^2 / \mu \varepsilon \]

(III-33)

\[ R_k = \rho k^2 \gamma_w / \mu \]

(III-37)

\[ C_c = 0.2 \]

(III-40)

\[ a_k = 0.87 \]

(III-29)

\[ \sigma_\varepsilon = 1.3 \]

(III-27)
\[ \text{Ri}_c = \frac{k^2 W}{\varepsilon \tau^2} \frac{\partial (rW)}{\partial r} \]  

(III-39)

\[ G = \nu_c [2\left( \frac{\partial V}{\partial r} \right)^2 + \frac{1}{r^2} \frac{\partial V}{\partial \theta} + \frac{1}{r^2} \frac{\partial V}{\partial \phi} + \left( \frac{\partial U}{\partial z} \right)^2 + \left( \frac{\partial U}{\partial r} \right)^2 + \left( \frac{\partial U}{\partial \phi} \right)^2 \]  

+ \left( \frac{1}{r^2} \frac{\partial M}{\partial \theta} \right)^2 + \left( \frac{1}{r^2} \frac{\partial M}{\partial \phi} + \frac{r}{r^2} \frac{\partial (W/r)}{\partial z} \right)^2 \]  

(III-106)

The three-dimensional conservation equations in the modified isotropic model for swirl flows can be summarized in Table III-3. This table is comparable to the results given in Table III-1 for two-dimensional flow except that the drag term appearing in the two-dimensional angular momentum equation does not exist in the three-dimensional equation. In this model the isotropy of the exchange coefficient \( \Gamma_\phi \) is assumed.

### 3.7.2 Conservation Equations in the Nonisotropic Model

In this subsection the conservation equations in the nonisotropic model, which includes the continuity equation, momentum equations and a nonisotropic \( k-\varepsilon \) turbulence model, are extended from the case of two independent variables to three independent variables. In this three-dimensional model, the isotropic assumption of \( \Gamma_\phi \) was eliminated. The general form is the same as equation (III-99), and the continuity equation is equation (III-100) as discussed in the previous subsection. Other individual equations are given below.

Radial momentum equation \((\phi=V, \Gamma_\phi=\nu_{rz})\) is an extension of equation (III-44):
Table III-3. Three-Dimensional Conservation Equations with the Isotropic Model.

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$\Gamma_\phi$</th>
<th>$S_\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
U & \quad \mu_{\text{eff}} = -\frac{\partial p}{\partial z} + \rho g_z \\
& \quad + \frac{1}{r} \frac{\partial}{\partial r} \left( \tau_{\text{eff}} \frac{\partial U}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \mu_{\text{eff}} \frac{\partial U}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( \mu_{\text{eff}} \frac{\partial U}{\partial z} \right) \\
V & \quad \mu_{\text{eff}} = -\frac{\partial p}{\partial r} + \mu \frac{V}{r} - 2\mu_{\text{eff}} \frac{V}{r} - 2 \frac{\mu_{\text{eff}} \partial W}{\partial \theta} \\
& \quad + \frac{1}{r} \frac{\partial}{\partial r} \left( \tau_{\text{eff}} \frac{\partial V}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \tau_{\text{eff}} \frac{\partial V}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( \mu_{\text{eff}} \frac{\partial V}{\partial z} \right) \\
rW & \quad \mu_{\text{eff}} = -\frac{\partial p}{\partial \theta} - 2 \frac{\partial}{\partial r} \left( \mu_{\text{eff}} \mu W \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \tau_{\text{eff}} \frac{\partial V}{\partial \theta} \right) \\
& \quad + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \mu_{\text{eff}} \frac{\partial (rW)}{\partial \theta} \right) + 2 \frac{\partial}{\partial \theta} \left( \mu_{\text{eff}} V \right) + \frac{\partial}{\partial z} \left( \mu_{\text{eff}} \frac{\partial W}{\partial z} \right) \\
\kappa & \quad \mu_{\text{eff}}/\sigma_k = \frac{G - \rho \varepsilon}{G} \\
\varepsilon & \quad \mu_{\text{eff}}/\sigma_\varepsilon = \frac{\varepsilon}{G} \left[ C_1 G - C_2 \left( 1 - C_3 R_4 \right) \rho \varepsilon \right]
\end{align*}
\]

where \( G = \mu \left[ 2 \left( \frac{\partial V}{\partial r} \right)^2 + \frac{1}{r} \frac{\partial W}{\partial r} + \frac{V}{r} \right]^2 + \frac{\partial U}{\partial r} + \left( \frac{\partial U}{\partial \theta} \right)^2 + \frac{1}{r} \frac{\partial U}{\partial \theta} + \frac{\partial W}{\partial \theta} \right]^2 \\
+ \frac{1}{r} \frac{\partial V}{\partial \theta} + \frac{\partial (rW)}{\partial \theta} \right]^2 \).
\[
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (r \psi^2) + \frac{1}{r} \frac{\partial}{\partial \theta} (r \psi \psi) + \frac{\partial}{\partial z} (\psi \psi) \right] = \frac{1}{r} \frac{\partial}{\partial r} (r \nu_{zz} \frac{\partial \psi}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{\nu_{zz}}{\sigma_{zz}} \frac{\partial \psi}{\partial \theta} \right) \\
+ \frac{\partial}{\partial z} \left( \frac{\nu_{zz}}{\sigma_{zz}} \frac{\partial \psi}{\partial z} \right) - \frac{\partial P}{\partial r} + \rho \left( \frac{\partial \psi}{\partial r} \right)^2 + \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{\sigma_{zz}} \psi_{zz} \frac{\partial \psi}{\partial r} \right)
\]

\[
+ \frac{\partial}{\partial \theta} \left( \frac{\nu_{zz}}{\sigma_{zz}} \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{zz}} \psi_{zz} \frac{\partial \psi}{\partial \theta} \right) - \frac{2 \nu_{zz}}{\sigma_{zz}} \frac{\partial \psi}{\partial \theta} - \frac{2}{\sigma_{zz}} \frac{\nu_{zz}}{r^2}
\]

\[
+ \frac{\partial}{\partial z} \left( \frac{\nu_{zz}}{\sigma_{zz}} \frac{\partial \psi}{\partial z} \right)
\]

(III-107)

Angular momentum equation \((\psi = r \psi, \Gamma_\phi = \nu_{rz})\) is an extension of equation (III-45):

\[
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (r \psi^2) + \frac{1}{r} \frac{\partial}{\partial \theta} (r \psi \psi) + \frac{\partial}{\partial z} (\psi \psi) \right] = \frac{1}{r} \frac{\partial}{\partial r} (r \nu_{zz} \frac{\partial \psi}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{\nu_{zz}}{\sigma_{zz}} \frac{\partial \psi}{\partial \theta} \right)
\]

\[
+ \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{zz}} \psi_{zz} \frac{\partial \psi}{\partial \theta} \right) - \frac{2 \nu_{zz}}{\sigma_{zz}} \frac{\partial \psi}{\partial \theta} - \frac{2}{\sigma_{zz}} \frac{\nu_{zz}}{r^2}
\]

(III-108)

Axial momentum equation \((\psi = U, \Gamma_\phi = \nu_{rz})\) is an extension of equation (III-46):

\[
\rho \left[ \frac{1}{r} \frac{\partial}{\partial r} (r \psi U) + \frac{1}{r} \frac{\partial}{\partial \theta} (r \psi U) + \frac{\partial}{\partial z} (\psi U) \right] = \frac{1}{r} \frac{\partial}{\partial r} (r \nu_{zz} \frac{\partial U}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{\nu_{zz}}{\sigma_{zz}} \frac{\partial U}{\partial \theta} \right)
\]

\[
+ \frac{\partial}{\partial z} \left( \frac{\nu_{zz}}{\sigma_{zz}} \frac{\partial U}{\partial z} \right) - \frac{\partial P}{\partial r} + \rho \frac{\partial}{\partial r} (r \nu_{zz} \frac{\partial U}{\partial r}) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{zz}} \psi_{zz} \frac{\partial U}{\partial \theta} \right)
\]

\[
+ \frac{1}{r} \frac{\partial}{\partial z} \left( \frac{1}{\sigma_{zz}} \psi_{zz} \frac{\partial U}{\partial z} \right) + \frac{\partial}{\partial \theta} \left( \frac{2}{\sigma_{zz}} \nu_{zz} \frac{\partial U}{\partial \theta} \right)
\]

(III-109)

Equation of turbulence kinetic energy \((\psi = k, \Gamma_\phi = \nu_{rz}/\sigma_k)\) is an extension of equation (III-47):
Equation of energy dissipation rate \((\phi = \epsilon, \Gamma = \mu_{rz}/\sigma_e)\) is an extension of equation (III-48):

\[
\rho \left( \frac{1}{r} \frac{\partial}{\partial r} (r \nu_{ck}) + \frac{1}{r^2} \frac{\partial}{\partial \theta} (r \nu_{0k}) \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu_{rz}}{\sigma_{r}} \frac{\partial \varepsilon}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{\theta}} \frac{\mu_{rz}}{\partial \varepsilon} \right)
\]

\[
+ \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{zz}} \frac{\mu_{rz}}{\partial \varepsilon} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{zz}} \frac{\mu_{rz}}{\partial \varepsilon} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{zz}} \frac{\mu_{rz}}{\partial \varepsilon} \right)
\]

\[
+ \text{const} - \rho \epsilon
\]

The above five equations and continuity equation (III-100) form a closed system with nonisotropic viscosity coefficient. This nonisotropic model can be viewed as a modification of the isotropic model. The other variables and empirical constants used in this model are given as follows:

\[
\mu_{rz} = \mu + C_{\mu} \rho k^2/\epsilon \quad (\text{III-50})
\]

\[
\nu_{rz} = \sigma_{rz}/\sigma_{r}\theta
\]

\[
\nu_{r\theta} = \sigma_{rz}/\sigma_{r\theta}
\]

\[
\nu_{r\theta} = \sigma_{rz}/\sigma_{rr}
\]

\[
\nu_{\theta\theta} = \sigma_{rz}/\sigma_{\theta\theta}
\]

\[
\nu_{zz} = \sigma_{rz}/\sigma_{zz}
\]

\[
\sigma_{r\theta} = \sigma_{\theta\theta} = \sigma_{rr} = \sigma_{zz} = 1.0 \quad \text{in bulk region} \quad (\text{III-58})
\]

\[
\sigma_{r\theta} = 1 + 2S_{r}^{1/3} \quad \text{in jet zone} \quad (\text{III-56})
\]

\[
\sigma_{\theta\theta} = \sigma_{rr} = \sigma_{zz} = 0.7 \quad \text{in jet zone} \quad (\text{III-57})
\]
The conservation equations in this three-dimensional nonisotropic model are tabulated in Table III-4.

3.7.3 Boundary Conditions for Three-Dimensional Equations

We have discussed the boundary conditions for the two-dimensional conservation equations previously. For the three-dimensional flowfield in an agitated vessel, we also need to consider the boundary conditions in the $\theta$-direction. Due to symmetry, a quarter of an agitated vessel should be selected as our calculation domain, and variables on one boundary are equal to the other. This will be discussed in detail in Section 3.9 Boundary Conditions in Numerical Representations. The values of variables on baffles are zero due to the no slip condition as discussed previously.

3.7.4 Three-Dimensional Discretization Equations

The two-dimensional general discretization equation was obtained by integrating equation (III-59) with respect to $r$ and $z$ from $w$ to $e$ and $b$ to $t$ over the finite domain in Figure III-2 in the first step of the
Table III-4. Three-Dimensional Conservation Equations with the Nonisotropic Model.

<table>
<thead>
<tr>
<th>φ</th>
<th>γ_φ</th>
<th>S_φ</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

\[
U_{rz} = - \frac{\partial P}{\partial z} + \rho g_z + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial U_{rz}}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{rz}} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \frac{1}{\sigma_{rz}} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{\sigma_{rz}} \right)
\]

\[
V_{rz} = \frac{\partial P}{\partial \theta} + \frac{\partial (\rho w)^2}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial V_{rz}}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \frac{1}{\sigma_{rz}} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{\sigma_{rz}} \right)
\]

\[
rW_{rz} = \frac{\partial P}{\partial \theta} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial (\rho w)^2}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{rz}} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \frac{1}{\sigma_{rz}} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{\sigma_{rz}} \right)
\]

\[
k_{rz/\alpha_k} = \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \frac{1}{\sigma_{rz}} \right)
\]

\[
\varepsilon_{rz/\alpha_\varepsilon} = \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \frac{1}{\sigma_{rz}} \right) + \frac{1}{r} \frac{\partial}{\partial \phi} \left( \frac{1}{\sigma_{rz}} \right)
\]

where \( G_{non} = \mu_{rz} \left( \frac{2}{\sigma_{rr}} \left( \frac{\partial \nu}{\partial \theta} \right)^2 + \frac{1}{\sigma_{rz}} \left( \frac{\partial \nu}{\partial \theta} \right)^2 + \nu \left( \frac{\partial \nu}{\partial \theta} \right)^2 \right) + \frac{1}{\sigma_{r\theta}} \left( r \frac{\partial \nu}{\partial \theta} \right) + \frac{1}{\sigma_{r\theta}} \left( \frac{\partial \nu}{\partial \theta} \right)^2 + \frac{1}{\sigma_{r\phi}} \left( \frac{\partial \nu}{\partial \phi} \right)^2 + \frac{1}{\sigma_{r\phi}} \left( \frac{\partial \nu}{\partial \phi} \right)^2 + \frac{1}{\sigma_{r\phi}} \left( \frac{\partial \nu}{\partial \phi} \right)^2 \)
discretization procedure. The result has been shown by equation (III-77). Similarly, the three-dimensional general discretization equation can be obtained with an additional integration with respect to θ from s to n over the finite domain shown in Figure III-6. This general discretization equation is written as follows:

\[ C_p\Phi = C_T\Phi + C_B\Phi + C_E\Phi + C_W\Phi + C_N\Phi + C_S\Phi + C_{S\Phi} \]  

(III-113)

where the subscripts N and S represent the north and south neighboring points of the central grid point P along the 0-coordinate, respectively. The locations of the grid points and surfaces of the finite domain in the r-θ plane are illustrated in Figure III-7.

Equation (III-113) illustrates that the variable of any grid point will be affected by its six neighbors by means of the corresponding coefficients, which are

\[ C_T = A_T \left( \frac{r_e + r_s}{2} \right) \Delta r \Delta \theta \]  

(III-114a)

\[ C_B = A_B \left( \frac{r_e + r_s}{2} \right) \Delta r \Delta \theta \]  

(III-114b)

\[ C_E = A_E r_e \Delta \theta \Delta z \]  

(III-114c)

\[ C_W = A_W r_w \Delta \theta \Delta z \]  

(III-114d)

\[ C_N = A_N \Delta r \Delta z \]  

(III-114e)

\[ C_S = A_S \Delta r \Delta z \]  

(III-114f)

\[ C_P = C_T + C_B + C_E + C_W + C_N + C_S - S_{41} \left( \frac{r_e + r_s}{2} \right) \Delta r \Delta \theta \Delta z \]  

(III-114g)

\[ C_{S\Phi} = S_{41} \left( \frac{r_e + r_s}{2} \right) \Delta r \Delta \theta \Delta z \]  

(III-114h)

where
Figure III-6. Three-dimensional finite domain for a main grid point.
Figure III-7. Finite domain in the r-θ plane.
The Peclet numbers in the above six equations are given by:

\[ N_{pt} = \frac{\rho U_t}{(\Gamma_{\phi_t}/\delta z_t)}, \quad N_{pb} = \frac{\rho U_b}{(\Gamma_{\phi_b}/\delta z_b)} \]  
(III-68)

\[ N_{pe} = \frac{\rho V_e}{(\Gamma_{\phi_e}/\delta r_e)}, \quad N_{pw} = \frac{\rho V_w}{(\Gamma_{\phi_w}/\delta r_w)} \]  
(III-73)

\[ N_{pn} = \frac{\rho W_n}{(\Gamma_{\phi_n}/r_n \delta \theta_n)}, \quad N_{ps} = \frac{\rho W_s}{(\Gamma_{\phi_s}/r_s \delta \theta_s)} \]  
(III-117)

The interface \( \Gamma_{\phi} \)'s in the above equations may be expressed in terms of grid-point \( \Gamma_{\phi} \)'s. One typical example is written as follows:

\[ \Gamma_{\phi_e} = \left( \frac{x_e(1 - f_e)}{x_e^{\phi P}} + \frac{x_e f_e}{x_e^{\phi E}} \right)^{-1} \]  
(III-74)

where \( f_e = \delta r_e^+ / \delta r_e \). There are similar expressions of \( \Gamma_{\phi_w}, \Gamma_{\phi_n}, \Gamma_{\phi_s}, \Gamma_{\phi_t}, \) and \( \Gamma_{\phi_b} \).

It should be noted that all the above expressions are formulated for the general differential equation (III-99) based on the finite domain as shown in Figure III-6. They are also applicable for the cases using staggered subdomains, such as \( U, V, \) etc., if appropriate changes in subscripts representing the grid points and interfaces have been made. The
grid points in the main finite domain should be treated as the interfaces in the staggered finite domains, and the interfaces of main domain should become the grid points for the staggered domains. Using this information and following the procedure used in Section 3.6, the discretized equations for pressure, pressure correction and velocities have been derived. They may be written as follows:

**Pressure equation:**

\[
C_p P_p = C_T P_T + C_B P_B + C_E P_E + C_W P_W + C_N P_N + C_S P_S + C_{SP} \tag{III-118}
\]

where

\[
C_T = \frac{1}{c_c} \left( \frac{r_e + r_w}{2} \right) \left( \frac{r_e + r_w}{2} \Delta x \Delta y \right) \tag{III-119a}
\]

\[
C_B = \frac{1}{c_b} \left( \frac{r_e + r_w}{2} \right) \left( \frac{r_e + r_w}{2} \Delta x \Delta y \right) \tag{III-119b}
\]

\[
C_E = \frac{1}{c_e} (r_e \Delta x \Delta z) (r_e \Delta y \Delta z) \tag{III-119c}
\]

\[
C_W = \frac{1}{c_w} (r_w \Delta x \Delta z) (r_e \Delta y \Delta z) \tag{III-119d}
\]

\[
C_N = \frac{1}{c_n} (r_e \Delta x \Delta z) (r_e \Delta x \Delta z) \tag{III-119e}
\]

\[
C_S = \frac{1}{c_s} (r_e \Delta x \Delta z) (r_e \Delta x \Delta z) \tag{III-119f}
\]

\[
C_p = C_T + C_B + C_E + C_W + C_N + C_S \tag{III-119g}
\]

\[
C_{SP} = -\rho \left( \hat{U}_e - \hat{U}_b \right) \left( \frac{r_e + r_w}{2} \right) \Delta x \Delta y \Delta \theta + \rho \left( \tau_e \hat{V}_e - \tau_w \hat{V}_w \right) \Delta \theta \Delta z \tag{III-119h}
\]

The coefficients such as \( C_e, C_w, \) etc. in the right hand sides of equations (III-119 a-f) can be calculated from equation (III-114 a-f) in the version
for the staggered finite domains. The hat velocity components, e.g. \( \hat{U}_t \), in equation (III-119h) are given as follows:

\[
\begin{align*}
\hat{U}_t &= \frac{1}{C_t} (\Sigma_{nb} U_{nb} + C_{S\phi}) \\
\hat{U}_b &= \frac{1}{C_b} (\Sigma_{nb} U_{nb} + C_{S\phi}) \\
\hat{V}_e &= \frac{1}{C_e} (\Sigma_{nb} V_{nb} + C_{S\phi}) \\
\hat{V}_w &= \frac{1}{C_w} (\Sigma_{nb} V_{nb} + C_{S\phi}) \\
\hat{W}_n &= \frac{1}{C_n} (\Sigma_{nb} (tW)_{nb} + C_{S\phi}) \\
\hat{W}_s &= \frac{1}{C_s} (\Sigma_{nb} (tW)_{nb} + C_{S\phi})
\end{align*}
\]

It should be noted that the contents in the above brackets have the same meaning, but are not the same thing.

**Velocity-correction equations:**

The velocity-correction equations for three-dimensional flows are extensions of equations (III-93,94,95,96) and are listed as follows:

\[
\begin{align*}
U_t &= U_t^* + \frac{1}{C_t} (P_P' - P_P') \left( \frac{r_e + r_w}{2} \Delta r \Delta \phi \right)_t \\
U_b &= U_b^* + \frac{1}{C_b} (P_B' - P_P') \left( \frac{r_e + r_w}{2} \Delta r \Delta \phi \right)_b \\
V_e &= V_e^* + \frac{1}{C_e} (P_W' - P_P') \left( r_e \Delta \phi \right)_e \\
V_w &= V_w^* + \frac{1}{C_w} (P_W' - P_P') \left( r_e \Delta \phi \right)_w \\
W_n &= W_n^* + \frac{1}{C_n} (P_W' - P_N') \left( \Delta r \Delta z \right)_n \\
W_s &= W_s^* + \frac{1}{C_s} (P_W' - P_P') \left( \Delta r \Delta z \right)_s
\end{align*}
\]
where the starred velocity field can be obtained from the following discretized momentum equations:

\[ C_T \mathbf{U}^* = \Sigma_{nb} \mathbf{U}_{nb}^* + C_S^\phi + (P^*_P - P^*_T)(\frac{\mathbf{r}_e + \mathbf{r}_w}{2}) \Delta x \Delta \theta \]  

(III-122a)

\[ C_B \mathbf{U}^*_b = \Sigma_{nb} \mathbf{U}_{nb}^* + C_S^\phi + (P^*_B - P^*_P)(\mathbf{r}_e \Delta x \Delta \theta)_b \]  

(III-122b)

\[ C_E \mathbf{V}^*_e = \Sigma_{nb} \mathbf{V}_{nb}^* + C_S^\phi + (P^*_P - P^*_E)(\mathbf{r}_e \Delta x \Delta \theta)_e \]  

(III-122c)

\[ C_W \mathbf{V}^*_w = \Sigma_{nb} \mathbf{V}_{nb}^* + C_S^\phi + (P^*_P - P^*_W)(\mathbf{r}_e \Delta x \Delta \theta)_w \]  

(III-122d)

\[ C_N (\tau W)_n^* = \Sigma_{nb} (\tau W)_{nb}^* + C_S^\phi + (P^*_P - P^*_N)(\Delta x \Delta \theta)_n \]  

(III-122e)

\[ C_S (\tau W)_b^* = \Sigma_{nb} (\tau W)_{nb}^* + C_S^\phi + (P^*_P - P^*_S)(\Delta x \Delta \theta)_b \]  

(III-122f)

where \( C_S^\phi \) represents the coefficient of the source term, \( S^\phi \), which excludes the pressure gradients, in the momentum equations. The symbol \( C_{nb} \) means the neighboring coefficients, i.e., \( C_e, C_w, \) etc. All these coefficients can be calculated from the suitable versions of equations (III-114 a-h). The superscript * is used to indicate the latest iterated values. The velocity components obtained from equation (III-122) will be used in equation (III-121) to obtain the corrected velocity field for the next iteration. The pressure-corrections appearing in equation (III-121) is obtained from the pressure-correction equation discussed below.

Pressure-correction equation:

\[ C_P^p \mathbf{P}^{'p} = C_T^T \mathbf{P}^{'T} + C_B^B \mathbf{P}^{'B} + C_E^E \mathbf{P}^{'E} + C_W^W \mathbf{P}^{'W} + C_N^N \mathbf{P}^{'N} + C_S^S \mathbf{P}^{'S} + C_S^\phi \]  

(III-123)
where all the coefficients except $C_{S^f}$ are calculated from equations (III-119 a-g), which are established for the pressure equation (III-118).

The $C_{S^f}$ in the above equation is

$$C_{S^f} = -\rho \left( w_e^* - w_s^* \right) \frac{r_e + r_w}{2} \Delta \theta \Delta z + \rho \left( r_e V_e^* - r_w V_w^* \right) \Delta \theta \Delta z$$

(III-124)

The right hand side of this equation is the finite difference version of the continuity equation. When velocity field is correct, equation (III-124) will become zero so that the continuity equation is satisfied. Therefore, this equation will provide the criterion of convergence of the iterations.

Before we step into the next section in which the numerical calculation method will be discussed, a brief summary is in order. In the earlier part of this chapter, we used four fundamental partial differential equations, i.e., the continuity equation and three momentum equations, to describe the flow in the mixing tank. However, they did not form a closure system for the turbulent flow, and hence the two-equation turbulence models were incorporated. Accordingly, we had six simultaneous differential equations, and they were expressed in the same form. Performing the integral method on the finite control volumes for this general differential equation, we obtained the general discretization equation, which can be used to stand for the continuity equation, pressure equation, pressure-correction equation, momentum equations, and other transport-property equations such as $k$-equation and $\varepsilon$-equation. Since the pressure field is also a property in the momentum equations, we derived the pressure equation and pressure-correction equation from the continuity equation and momentum equations. The continuity equation, pressure
equation and pressure-correction equation were not independent. The continuity equation became part of the pressure-correction equation and played the role as the criterion for convergence. The detailed steps of the iterative solution of these algebraic equations will be presented in the next section.

3.8 Calculation Method

In the last section we have presented both two- and three-dimensional discretized forms of the general transport equation. In the two-dimensional case, equation (III-77) is used to solve for the angular velocity, pressure and pressure-correction as well as turbulence kinetic energy and its dissipation rate. Its "staggered" version, i.e., equations (III-80) and (III-81), are used to solve for the axial and radial velocity components. In the three-dimensional case, pressure, pressure correction, turbulence kinetic energy, and dissipation rate are obtained from equation (III-113), and the three velocity components are obtained by solving the "staggered" equations (III-122a-f). In this section, two computational procedures for solving the sets of algebraic equations will be described. These are the SIMPLE and SIMPLER algorithm. The SIMPLE algorithm has been extensively used and has served well for the solution of simultaneous transport equations. Its revised version called SIMPLER will also be used. Both of these methods use the Tri-Diagonal Matrix Algorithm (TDMA) for solving the individual equation, and in the next subsection this algorithm will be described briefly.
3.8.1 TDMA with Sweep Method

Equations (III-77) and (III-113) represent a set of linear algebraic equations. The matrix of the coefficients of this set of equations can be arranged to have a band of non-zero coefficients along the diagonal. Special algorithms to solve these types of algebraic equations have been developed, and they use Gaussian elimination. One algorithm is known as the Tri-Diagonal Matrix Algorithm (TDMA), which applies to matrices with non-zero coefficients on three diagonals. The algorithm begins with a finite difference equation with the following form:

$$a_i \phi_i = b_i \phi_{i+1} + c_i \phi_{i-1} + d_i \quad \text{for } i=1,2,...,N \quad \text{(III-125)}$$

where \(i\) denotes the numbered grid points with points 1 and \(N\) representing the boundary points. \(c_1=0\) and \(b_N=0\) for \(i=1\) and \(i=N\) are specified such that the tridiagonal form of the matrices can be obtained. Gaussian elimination can be applied to the equation with the form of equation (III-125), and a set of recursion relations can be obtained which are given below.

$$M_i = b_i/(a_i - c_i M_{i-1}) \quad \text{for } i=1,2,...,N \quad \text{(III-126)}$$

$$N_i = (d_i + c_i N_{i-1})/(a_i - c_i M_{i-1}) \quad \text{for } i=1,2,...,N \quad \text{(III-127)}$$

where \(c_1=0\) and for \(i=1\) these equations are:

$$M_1 = b_1/a_1 \quad \text{(III-128)}$$

$$N_1 = d_1/a_1 \quad \text{(III-129)}$$

All of the values of \(M_i\) and \(N_i\) can be computed for \(i=1,2,...,N\). Then the values of \(M_i\) and \(N_i\) are then used to compute the values of \(\phi_i\) using the following equation.
\[ \phi_i = M_i \phi_{i+1} + N_i \quad \text{for } i=N-1,N-2,...,2,1 \quad (III-130) \]

where

\[ \phi_N = N_N \quad (III-131) \]

This is a very popular and simple procedure for the solution of the one-dimensional discretization equation.

Although the TDMA is a solution technique for one-dimensional cases, it can be used to solve multi-dimensional finite difference equations with the help of a simple iterative method. For the two-dimensional case, we can apply the TDMA in the \( z \)-direction if we consider \( \phi_E \) and \( \phi_W \) in the \( r \)-direction to be known. The latest iterated values of \( \phi_E \) and \( \phi_W \) are used, and equation (III-77) can be written as

\[ C_p \phi_p = C_T \phi_T + C_B \phi_B + (C_E \phi_E^* + C_W \phi_W^* + C_S \phi) \quad (III-132) \]

which is of the same form as equation (III-125) with \( d_i \) given as:

\[ d_i = C_E \phi_E^* + C_W \phi_W^* + C_S \phi \quad (III-133) \]

Similarly, we can apply the TDMA in the \( r \)-direction if the last iterated values of \( \phi_T \) and \( \phi_B \) are used in equation (III-77), which now can be written as:

\[ C_p \phi_p = C_E \phi_E + C_W \phi_W + (C_T \phi_T^* + C_B \phi_B^* + C_S \phi) \quad (III-134) \]

to match the form of equation (III-125).

Accordingly, the two-dimensional finite difference equations like equation (III-77) can be solved by the successive application of the TDMA in the \( z \) and \( r \) directions. Sweeping along the \( r \)-direction and \( z \)-direction alternatively with a convergence criterion, a solution for \( \phi_p \) can be obtained. We can first choose a grid line along the \( z \) direction, use the
latest values of $\phi$ on the two $r$-direction neighboring lines, and solve for all $\phi$'s along the chosen line by the TDMA. This procedure will be followed for all grid lines in the $z$ direction. Then we choose the grid lines in the $r$-direction, and use the latest values of $\phi$ on the two corresponding $z$-direction neighboring lines, and solve for all $\phi$'s along the chosen line by the TDMA. This method can be extended to three-dimensional equations of the form of equation (III-113) where all three coordinate axes are swept alternatively.

The above scheme, in which the TDMA is applied to one direction with an interactive method sweeping along the different directions one after another, can provide a faster convergence than a pure iterative method such as the Gauss-Seidel method according to Patankar(40). This is because all the boundary conditions from the ends of the grid lines along different directions are immediately brought into the interior of the calculation domain by the TDMA(40). This is the reason why the TDMA with sweep method is adopted in this work.

3.8.2 SIMPLE Algorithm(42)

The previous discussion showed how an individual algebraic equation represented by equation (III-77) or (III-113) could be solved by the TDMA with sweep method. Now, we will present efficient ways to solve the coupled equations for rapid convergence. The first method is the popular SIMPLE algorithm, and the sequence of calculation for this algorithm is as follows:

(1) Start with a guessed pressure field.

(2) Guess the values of $k$ and $\varepsilon$ for the first run of calculation

(3) Calculate all $I_\phi$'s.
(4) Calculate the coefficients, C's, in the momentum equations (III-122 a-f).

(5) Obtain $V^*$, $W^*$ and $U^*$ by solving the momentum equations (III-122 a-f).

(6) Calculate the coefficients for the pressure-correction equation (III-123). If the source term, equation (III-124), is equal to zero, the convergence of the calculation is reached.

(7) Solve the $P'$ equation (III-123) to obtain all pressure-corrections.

(8) Obtain the pressure field by adding $P'$ to $P^*$, equation (III-92). Underrelaxation might be needed, i.e., $P = P^* + \beta_p P'$ where underrelaxation factor for pressure $\beta_p$ is in a range from 0 to 1. The corrected $P^*$ will become a new guess pressure $P^*$ for next iteration.

(9) Correct $V$, $W$ and $U$ by use of velocity-correction equations (III-121 a-f).

(10) Calculate all coefficients and constants in the $k$- and $\epsilon$-equation, and solve them.

(11) Return to step 3 for the next run of iteration.

The acronym SIMPLE stands for Semi-Implicit Method for Pressure Linked Equations(40). In this algorithm an initial guess for pressure field and turbulence field, i.e., $P$, $k$ and $\epsilon$, are needed for iterative computations.

A revision of the SIMPLE algorithm which provides a different way to obtain pressure field is called SIMPLER(40). This algorithm will be discussed below.

3.8.3 SIMPLER Algorithm(40)

In the SIMPLE algorithm the pressure-correction $P'$ of step 7 is used to obtain the pressure field by $P = P^* + \beta_p P'$ of step 8 in the SIMPLE algorithm. In its revised version, the SIMPLER algorithm, the pressure equation
(1) Start with a guessed velocity field.
(2) Guess the values of \( k \) and \( \varepsilon \) for the first run of calculation
(3) Calculate all \( \Gamma_\phi \)'s.
(4) Calculate the coefficients, \( C \)'s, in the momentum equations (III-122 a-f).
(5) Calculate the hat velocities \( \hat{V} \), \( \hat{W} \) and \( \hat{U} \) from equations (III-120 a-f) with the coefficients obtained in the preceding step and the latest values of the corresponding neighbor velocity field, \( V_{nb} \), \( W_{nb} \) and \( U_{nb} \).
(6) Calculate the coefficients for the pressure equation (III-118).
(7) Obtain the pressure field by solving the \( P \) equation (III-118).
(8) Treating the above pressure field as \( P^* \), solve the momentum equations (III-122 a-f) for \( V^* \), \( W^* \) and \( U^* \).
(9) Calculate from equation (III-124) the source term, \( C_{S\phi} \), in the pressure-correction equation (III-123). If it is zero, convergence of the calculation has been reached.
(10) Solve the \( P' \) equation (III-123) to obtain all pressure-corrections.
(11) Correct \( V \), \( W \) and \( U \) by use of velocity-correction equations (III-121 a-f).
(12) Calculate all coefficients and constants in the \( k \)- and \( \varepsilon \)-equation, and solve them.
(13) Return to step 3 for the iteration.

Unlike the original algorithm, which requires a reasonable initial guess of the pressure field, the SIMPLER algorithm needs a reasonable
initial estimate of the velocity field. In many problems, an estimate of a reasonable initial velocity field is easier to obtain than an estimate of pressure field. Therefore, the pressure field calculated in the SIMPLER algorithm may be closer to the correct pressure field, and fewer iterations may be required for the converged solution of the same criteria. However, the initial guess for turbulence parameters is still required, and this may hurt the contribution made by the pressure field in turbulent flows. Also, the SIMPLER algorithm needs to solve one more equation, i.e., pressure equation, than the SIMPLE algorithm; and the SIMPLER algorithm uses more computer storage than SIMPLE. Thus, whether the SIMPLER algorithm can obtain converged solution with less computer time than the SIMPLE algorithm should be problem-dependent. Anderson, et al.(43) reported that in most cases a reduction in computer time of 30-50% is obtained even though SIMPLER required about 30% more computation effort per iteration than the SIMPLE algorithm. In this study, both algorithms are applied in two-dimensional simulations for the turbulent flow in agitated vessel in which no accurate initial estimate of turbulence field, velocity field, or pressure field existed. The comparison of the two-dimensional computations for the turbulent flow in an agitated vessel with these two algorithms will be reported in next chapter. The computed results from the two-dimensional solutions will be used for the initial estimate of the three-dimensional flowfield.

3.9 Boundary Conditions in Numerical Representations

We have presented all the elements needed for a numerical solution except how the boundary conditions are incorporated in the solution procedure. The boundary conditions for the governing equations were given
in previous sections for the two-dimensional axisymmetric and three-dimensional flowfields. In this section, we will discuss how to express the boundary conditions in the finite domain scheme.

In section 3.5, we mentioned that the boundary conditions for axial and tangential velocity components on the top and bottom of the impeller had values from a material balance and solid rotation of the impeller. Here we can use the following equations to provide these boundary conditions:

\[ W(I,J) = W(I,J_R) \frac{r(J)}{r(J_R)} \quad \text{for } I=I_T \text{ or } I=I_B \]  
\[ (III-135) \]

\[ U(I_T,J) = \alpha U(I_T+1,J) \]  
\[ (III-136) \]

and

\[ U(I_B,J) = \alpha U(I_B-1,J) \]  
\[ (III-137) \]

where subscript \( R \) means the radius of the impeller, and thus \( J_R \) indicates the impeller tip. The proportional constant \( \alpha \) can be obtained from the balance over the blade-swept region which is treated as a black box. The details about how to obtain \( \alpha \) are given in Appendix A. The introduction of the proportional constant \( \alpha \) guarantees that the overall balance will be satisfied for the entire blade-swept region. If the computed \( \alpha \) is equal to unity, the normal assumption of \( \partial U/\partial z = 0 \) is then numerically satisfied. The values of \( \alpha \) in Table A-1 were calculated from two-dimensional simulations, and they were not equal to unity. The average values of \( \alpha \) for three different tank systems will be used in three-dimensional simulations.

As for the boundary conditions in the \( \theta \)-direction, we need to pay special attention to them. Due to symmetry, a quarter of the mixing tank should be selected as our calculation domain. As shown in Figure
III-8(a), the no slip condition applies to wherever baffles locate, and variables on boundary $K=1$ are the same as those on $K=KPT$, i.e.,

$$
\phi_{K=1} = \phi_{K=KPT}
$$

and

$$
\phi_{K=KPT} = \phi_{K=1}
$$

Apparently these two boundary conditions are dependent. Therefore, we are in need of one more relation. To conquer this problem, we may turn to expand the calculation domain as shown in Figure III-8(b). According to the symmetry, we then have

$$
\phi_{K=1} = \phi_{K=KPT-2} \tag{III-138}
$$

and

$$
\phi_{K=KPT} = \phi_{K=3} \tag{III-139}
$$

where $\phi_{K=3}$ and $\phi_{K=KPT-2}$ are obtained from the lastest iteration.

When the boundary conditions are Neumann type, we need to construct an expression to relate the values of the variables of the boundary point to those of the neighboring interior grid point. A suitable finite form for $\partial \phi / \partial r=0$ and $\partial \phi / \partial z=0$ is

$$
\phi_B = \phi_I \tag{III-140}
$$

where subscripts B and I stand for the boundary point and its first neighboring point, respectively. Another method to reach the same goal in the numerical scheme is that the $\Gamma_{\phi}$ of the boundary control volume bounded by points B and I is artificially set equal to zero. The reason to do this is the fact that $\Gamma_{\phi}(\partial \phi / \partial x_i)$, where $x_i$ means any coordinate, always comes together in the transport equations. Thus, when we artificially set $\Gamma_{\phi}$ equal to zero, the term $\Gamma_{\phi}(\partial \phi / \partial x_i)$ will vanish in the calculations;
Figure III-8. Calculation domain in the $r-\theta$ plane.
this is also the result caused by the boundary conditions of the second kind, \( \frac{\partial \phi}{\partial x_i} = 0 \).

In this work, we also need to represent some boundary conditions in the inner positions of the tank, as shown in Figures III-1 and III-8(b), in the finite difference form. One of the most common and convenient methods to express these "internal" boundary conditions is to introduce a very big number (e.g. \( 10^{30} \)) in the discretization equation (III-113) so that any specified value of the variable can happen to be the solution of the equation at some internal grid point (40). We can set \( S_{\phi_1} \) and \( S_{\phi_2} \) for the point of interest as

\[
S_{\phi_1} = 10^{30} \phi_{p, \text{specified}} \quad \text{ (III-141a)}
\]

\[
S_{\phi_2} = -10^{30} \quad \text{ (III-141b)}
\]

and substitute them into equations (III-113) and (III-114) where the other terms become negligible. The discretization equation (III-113) then reduces to:

\[
-S_{\phi_2} \phi_p = S_{\phi_1} \phi_{p, \text{specified}}
\]

which leads to \( \phi_p = \phi_{p, \text{specified}} \), the result we pursue.

The idea of applying a big number is also applicable to the boundary conditions of \( \frac{\partial \phi}{\partial x_i} = 0 \) at internal grid points. For \( \frac{\partial \phi}{\partial x_i} = 0 \) we need to have \( \phi_p = \phi_{nb} \), where subscript nb means a neighboring point of the central grid point P (e.g. E, W, T, etc.), during iteration. We may set

\[
S_{\phi_1} = 10^{30} \phi_{nb} \quad \text{ (III-142a)}
\]

\[
S_{\phi_2} = -10^{30} \quad \text{ (III-142b)}
\]

Alternatively, we can let
\[ C_{nb} = 10^{30} \quad (III-143a) \]
\[ C_p = 10^{30} \quad (III-143b) \]

which will also result in \( \phi_p = \phi_{nb} \).

Using the methods described above, all boundary conditions in this study can be easily incorporated to the calculation. These include the second type of boundary conditions on outer boundary and the first and second type of boundary conditions at internal grid points in the calculation domain.

3.10 Summary

In this chapter, we proposed governing equations to describe the turbulent flow in agitated vessels. We started with the conservation equations which govern the turbulent flow in agitated vessels. We then pointed out that it was necessary to have a turbulence model to close the governing equations and to be able to obtain a solution, and we proposed two types of modified k-\( \varepsilon \) two-equation models. The boundary conditions associated with the conservation equations were also presented. The boundary conditions for rotating turbine included the tangential jet model and a material balance for the returning flow.

Also, a method of solution for these equations was presented. First, all the differential equations were arranged in a common form. Then using this form, a general discretization equation was obtained with the finite domain method. The TDMA with sweep method was applied to the general discretization equation, and the SIMPLE and SIMPLER algorithms were used to specify the order of solution of the discretization equations. The
approach began with the two-dimensional axisymmetric equations, and then they were extended to three dimensions. It was more convenient to begin the development of both differential and discrete equations in two-dimensional form, and to program step by step. Also, the two-dimensional solutions would provide a good initial estimate of variables for the three-dimensional program for more rapid convergence. In addition, the more economic algorithm between SIMPLE and SIMPLER, determined by comparing their CPU time required for the two-dimensional modeling, was used in three-dimensional computations. In next chapter, the results from both two- and three-dimensional computations will be presented and discussed.
3.11 References


CHAPTER IV

RESULTS AND DISCUSSION

4.1 Introduction

In this chapter we will begin by giving the results of the solution for the three-dimensional turbulent flowfield including the convergence and validity of the solution as established by comparison with experimental data. Also, the solution from the three-dimensional isotropic and nonisotropic simulation will be compared. Then we will present the results from the two-dimensional axisymmetric solutions and show the limitations associated with this approximation. The comparisons will include the results from four different two-dimensional models. In addition, there will be a discussion on the relation of this research to previous studies on the turbulent flow in agitated vessels. We will then discuss the numerical convergence and accuracy, and finally the SIMPLE and SIMPLER algorithms will be compared for efficiency in the numerical solution for this particular flowfield.

4.2 Three-Dimensional Simulation

In this section we will present the three-dimensional solution for the turbulent flowfield in three different stirred tank systems. As shown in Table IV-1, they are for an agitated vessel of the same size but with different impeller speeds and diameters. We will then verify the
Table IV-1. Three Stirred Tank Systems.

<table>
<thead>
<tr>
<th>Tank system</th>
<th>Impeller speed</th>
<th>Impeller diameter</th>
<th>Tank diameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>250 rpm</td>
<td>3 inches</td>
<td>11.5 inches</td>
</tr>
<tr>
<td>2</td>
<td>150 rpm</td>
<td>4 inches</td>
<td>11.5 inches</td>
</tr>
<tr>
<td>3</td>
<td>200 rpm</td>
<td>4 inches</td>
<td>11.5 inches</td>
</tr>
</tbody>
</table>
suitability of the nonisotropic model for the turbulent flow in stirred tanks by comparing the calculated results with the measured velocity profiles in the three stirred tank systems from Mulvahill (6, Chapter I). Also, Patterson and Wu's results (28, Chapter II) for the turbulence intensities and energy dissipation rates in the impeller stream of their agitated vessel will be used for qualitative comparison of turbulence field.

The SIMPLE algorithm was used for the solution of the governing equations for the turbulent flow in stirred tanks, and the two-dimensional simulation results were used for initial estimates in three-dimensional calculations. Following standard practice in the literature, the quantities were nondimensionalized as follows:

\[
\begin{align*}
r' &= r/(\frac{1}{2}D_i) \\
z' &= z/(\frac{1}{2}D_i) \\
V' &= V/(\pi ND_i) \\
W' &= W/(\pi ND_i) \\
U' &= U/(\pi ND_i) \\
k' &= k/(N^2D_i^2) \\
\varepsilon' &= \varepsilon/(N^2D_i^2)
\end{align*}
\]

The axial distance \( z \) is measured from the impeller plane with positive values above the plane and negative values below it. These dimensionless variables are used in all diagrams of this chapter. In this nondimensionalization, the impeller speed \( N \) and impeller diameter \( D_i \) are used because they are important impeller characteristics as discussed in
Chapter II. The concept of nondimensionalization is particularly important for initial estimates for $k$ and $\varepsilon$ in the calculation to obtain a solution of the turbulent flow in different stirred tank systems. The initial estimates for variables will be discussed in the section dealing with convergence.

4.2.1 Solution from Nonisotropic Model

In this subsection we will present the three-dimensional solution from the nonisotropic simulation. The variations of variables in the tangential direction, resulting from baffles, will be seen in this three-dimensional solutions.

4.2.1.1 Velocity Field Description

Figure IV-1 shows typical result for the velocity vectors on the $45^\circ$ plane, i.e. the $r-z$ plane centered between the baffles, in Tank System 1. It illustrates the circulation of the fluid in agitated vessels. The magnitude of the resultant velocity was obtained using $(V^2+U^2)^{1/2}$ and the direction was $\tan^{-1}(U/V)$. These velocity vectors were nondimensionalized by dividing by the impeller tip velocity $V_{\text{tip}}=\frac{N D_I}{\omega}$. As shown in the figure, the radial velocity components dominate in the impeller stream with the maximum magnitude of about $0.6V_{\text{tip}}$. The radial motion of the flow turns to the axial direction in the region near the wall. In this wall region the maximum magnitudes of the velocity are about $0.15V_{\text{tip}}$. In the regions near the top and bottom of the vessel, i.e. $z'\approx \pm 3.0$, radial motion is relatively dominant and the maximum magnitude of the velocity is about $0.1V_{\text{tip}}$. The flow in the regions near the centerline of the tank is mainly in the axial direction with the maximum magnitude of about $0.2V_{\text{tip}}$. 
Figure IV-1. The dimensionless velocity vectors on the 45° r-z plane in Tank System 1.
The velocity vectors are largest in the jet zone and relatively small in the bulk region.

It should be pointed out that the velocity vectors at the locations outside the jet zone are pointing toward the impeller stream. This shows that there is an entrainment of the fluid in the impeller stream. Also, we can see that the flow in the stirred tank is not symmetrical about the impeller plane. This is caused by the tank construction. There is a rotating impeller shaft and free surface in the upper half of the tank, but it is the tank bottom in the lower half. However, there is symmetry in the jet zone, especially in the region close to impellers. The rotating impeller dominates this region and overrides the effect from the flow in bulk regions.

Figure IV-2 is a typical top view of mean-flow velocity vectors on the r-θ plane at the axial position z' = 2.5 in Tank System 1. At this location, the flow is moving toward the centerline of the vessel. It also shows that the flow is mainly in the tangential direction except in the regions behind the baffles where a recirculating flow is found. This indicates that the fluid motion in agitated vessels is affected by the baffles and the flow is three-dimensional. The magnitude of the resultant velocity was obtained using \((W^2 + V^2)^{\frac{1}{2}}\) and the direction was \(\tan^{-1}(W/V)\). These velocity vectors were also nondimensionalized with \(V_{tip}\). The velocities in the tank wall region was found to be relatively small with magnitude of about 0.04 to 0.08\(V_{tip}\) compared to the maximum magnitudes of about 0.15\(V_{tip}\) away from the wall and centerline. The minimum velocities with magnitude of about 0.02\(V_{tip}\) were found in the regions close to the centerline of the tank where the flow is mainly in the axial direction as shown in Figure IV-1.
Figure IV-2. The dimensionless velocity vectors on the \( r-\theta \) plane at the location of \( z^* = 2.5 \) in Tank System 1.
4.2.1.2 Turbulence Field Description

In this subsection we will describe the turbulence field from the three-dimensional solutions of the turbulence kinetic energy and dissipation rate. Figure IV-3 presents the nondimensional turbulence kinetic energy on the r-θ plane at z' = 0, the plane of the impeller in Tank System 1. The turbulence kinetic energy close to the impeller tip is over ten times that in the regions away from the impeller. The variation of the turbulence energy along the θ-direction in the region close to the impeller is much smaller than the variation in the wall region. From Figure IV-3, we see that at r' = 1.3 the variation in the θ-direction is from 11.3 to 11.8 (or 4%) while the variation at r' = 3.33 is from 0.693 to 0.851 (or 19%). This shows that baffles make the flowfield in an agitated vessel become three-dimensional. Plots for the distribution of turbulence kinetic energy on the impeller plane in Tank System 2 and 3 are given in Figures B-1 and B-2 of Appendix B, and these show the same behavior.

The contours of the turbulence kinetic energy on the 45° r-z plane in Tank System 1 were drawn in Figure IV-4. The turbulence kinetic energy contours show that the values of k' in the bulk region of Tank System 1 are of the order of 0.2 which is significantly less than those in the impeller stream where the values of k' are about 5.0. It is worthwhile to notice that the values of k' along the tank wall show the continuation of the impeller jet, which is usually considered to become a wall jet after impinging on the wall. It is reasonable to find that the energy carried by the wall jet is smaller than the preceding impeller jet, since there is no energy source other than the rotating impeller.

From the contour map of Figure IV-4, we can also see that the values of turbulence kinetic energy at the centerline above the impeller plane are higher than those in the corresponding region below the impeller. This is
Figure IV-3. Turbulence kinetic energy on the r-θ plane at z' = 0, the impeller plane, in Tank System 1.
Figure IV-4. Contours of turbulence kinetic energy on the 45° plane in Tank System 1.
the energy from the rotating impeller shaft. Also, the contours at the tank bottom are different from those at the free surface. In addition, the contours are basically symmetrical in the jet zone, but become asymmetrical in the bulk region.

In Figure IV-5 the front-view and back-view of the block diagrams for the nondimensional turbulence kinetic energy are given on the 45° r-z plane for Tank System 1. The dominance of the impeller jet in the turbulence energy of agitated vessels cannot be expressed better than the mountain on the plot.

The contours and block diagrams of the turbulence kinetic energy on the 45° r-z plane in Tank System 2 and Tank System 3 are located in Figures B-3 to B-6 of Appendix B. They show comparable results that most of the turbulence energy is in the impeller stream, and the remaining energy in the bulk regions is relatively small. The turbulence energy is transferred from the impeller jet to the wall jet. These contour maps also show the symmetry in the jet zone and higher turbulence kinetic energy around the impeller shaft.

The nondimensional turbulence energy dissipation rate of the impeller jet on the r-θ plane in the three stirred tank systems are shown in Figure IV-6, Figure B-7, and Figure B-8, respectively. We find that the energy dissipation rate for the region close to the impeller tip is much higher than the dissipation rate in the regions away from the impeller. Most of the turbulence kinetic energy is consumed in the region near the impeller tip. The variation of the energy dissipation rate along the θ-direction matches the variation of the turbulence kinetic energy. It is worthwhile to point out that baffles also plays a role in consuming some turbulence kinetic energy as shown by the values of 1.02 near the baffles as compared to 0.72 on the 45° r-z plane.
Figure IV-5. Block diagrams of turbulence energy on the 45° plane in Tank System 1.
Figure IV-6. Energy dissipation rate of the impeller stream on the r-θ plane in Tank System 1.
The contours for the dissipation rates of turbulence kinetic energy on the 45° r-z plane in Tank System 1 are displayed in Figure IV-7. It is no surprise that the impeller stream accounts for most of the turbulence energy dissipation. In the rest of the agitated vessel, the dissipation rates of turbulence energy are relatively small, i.e. from 1.0 to 0.1 as compared to 4.0 to 32.0 in the impeller stream. This matches Patterson and Wu's observation(28, Chapter II).

From the contour map of Figure IV-7, we can also see that the wall region, especially near the impeller plane, dissipates more turbulence energy than the other regions of the tank except the jet zone. Impeller shaft region also consumes more turbulence energy than most of the bulk region. In summary, the distribution of energy dissipation rates follows the same pattern as the turbulence energy distribution.

The complete distribution of the turbulence energy dissipation rates in Tank System 1 can be more easily seen from the different views of block diagrams in Figure IV-8. As for the distribution of energy dissipation rates in Tank System 2 and Tank System 3, they are displayed in Figures B-9 to B-12. All of these plots are very similar to those for Tank System 1.

We have presented some typical results from the solution of the governing equations with the nonisotropic turbulence model. In the next section we will present a comparison of this solution with experimental data from Mulvahill(5, Chapter I) for velocities and from Patterson and Wu(28, Chapter II) for the turbulence parameters.
Figure IV-7. Contours of energy dissipation rates on the 45° plane in Tank System 1.
Figure IV-8. Block diagrams of dissipation rates on the 45° plane in Tank System 1.
4.2.2 Validation of Nonisotropic Model

In this section we will compare the three-dimensional solution from the nonisotropic simulation with experimental data. The discussion about the velocity field will be first, and this will be followed by the turbulence field.

4.2.2.1 Velocity Field Validation

In Figure IV-9 to IV-11 the variations in the three velocity components along the $\theta$-direction are given for the nonisotropic simulation, and these profiles are compared with Mulvahill's experimental data (6, Chapter I) at a $r$-$z$ location in the bulk region of each of the three tank systems. Additional comparisons are given in Figures IV-12 through IV-14 for the velocity profiles in the radial direction with Mulvahill's (6, Chapter I) data on the $45^\circ$ $r$-$z$ plane. As discussed below we will be able to conclude that the nonisotropic model fits the experimental data to within the accuracy of the data, and the nonisotropic simulation predicts the velocity field in agitated vessels.

In Figure IV-9, comparisons of the dimensionless radial velocities $V'$ in the $\theta$-direction for three values of $r$ and $z$ are made with experimental data for three tank systems. The velocity profiles for $V'$ generally fit the experimental data within the accuracy of the data. At these locations the radial velocity $V'$ is negative which means that the flow is away from the tank wall and toward to the centerline of the vessels. From the three plots in Figure IV-9, we can see that the variation of radial velocity along the $\theta$-direction is significant. Baffles are located at $\theta'=0$ and $\theta'=90^\circ$, and the impeller is rotating counter-clockwise. From the shape of the curves, we find the largest changes occur in the regions near where baffles are located.
Figure IV-9. Radial velocity profiles along the θ-direction.

- Tank System 1
- V' = 3.48
- z' = 2.0

- Tank System 2
- V' = 2.6
- z' = 1.9

- Tank System 3
- V' = 1.7
- z' = 1.6
Figure IV-10. Tangential velocity profiles along the θ-direction.
Figure IV-11. Axial velocity profiles along the $\theta$-direction.
Figure IV-12. Radial velocity profiles along the r-direction on the 45° plane.
Figure IV-13. Tangential velocity profiles along the r-direction on the 45° plane.
Figure IV-14. Axial velocity profiles along the r-direction on the 45° plane.
In Figure IV-10, comparisons of the dimensionless tangential velocities $W'$ along the $\theta$-direction for three values of $r$ and $z$ are made with the experimental data for the three tank systems. The velocity profiles for $W'$ generally fit the experimental data within the accuracy of the data, and the largest deviation occurs in the region close to the baffles in Tank System 2. This is probably due more to interference by the hot wire anemometer probe in the velocity measurement rather than a model deficiency. In the center plot of Figure IV-10, we find the calculated tangential velocities in the range from $0^\circ$ to $10^\circ$, measured from baffles, become negative, and this shows recirculating flow behind baffles. This phenomenon is reasonable, but is not confirmed by the experimental data. The variation of tangential velocity in the $\theta$-direction is the largest in Tank System 2 and the smallest in Tank System 3.

In Figure IV-11, comparisons for the dimensionless axial velocity $U'$ profiles along the $\theta$-direction are made with the experimental data at a value of $r$ and $z$ for each of the three tank systems. The variation of the axial velocity along the $\theta$-direction is also distinct which illustrates the three-dimensional character of the flow. In the region close to tank wall, e.g. $r'=3.46$ in Tank System 1 and $r'=2.6$ in Tank System 2, the effect of baffles turning the flow is seen. Also, the axial velocity at this location close to the front face of baffle is higher than the axial velocity on the back side of the baffle.

The previous results and discussion have shown the three-dimensional character of the flow, and that the theoretical solution of the governing equations with the nonisotropic turbulence model agrees with the experimental data for variation in the $\theta$-direction. We will now continue the comparison of the velocity profiles with the data of Mulvahill.
(6, Chapter I) on the 45° plane, i.e. the r-z plane centered between the two baffles.

In Figure IV-12, the radial velocity $V'$ profiles are compared with experimental data along the r-direction for three different axial positions in the bulk region of the three stirred tank systems. The measured radial velocities are negative, and this shows that the flow is recirulating back from the tank wall to the centerline. The calculated radial velocities have the same behavior in the three stirred tank systems. In Tank Systems 2 and 3, the numerical results match the experimental data within the accuracy of the data. In Tank System 1, however, there is a noticeable discrepancy between the experimental data and computed velocity at $r'=1.0$ to 1.5. There is no obvious explanation for this discrepancy, and it is the largest observed in all of the comparisons with experimental data. It could be a problem with probe interference or it could be associated with the accuracy of the numerical solution or a model parameter.

In Figure IV-13, the tangential velocity $W'$ profiles are compared with experimental data along the r-direction for three tank systems. The numerical results agree with the data, and the largest deviation occurs near the tank wall where there was possible probe interference with the velocity measurement. The calculated tangential velocities are consistently slightly higher than the experimental data which could indicate a requirement for the fine tuning of some turbulence model parameter.

In Figure IV-14 the axial velocity $U'$ profiles are compared with experimental data in the r-direction for three different axial positions in three stirred tank systems. The numerical profiles show that the flow is moving upward near the tank wall and moving downward in the region away
from the wall. These calculated results match the data in the regions where \( r' > 1.5 \), i.e. about midway between centerline and tank wall. In the regions of \( r' < 1.5 \), i.e. close to the centerline of the tank, the calculated axial velocities are negative, and they deviate from the experimental data. The computed results show the flow moving toward the impeller zone sooner than the experimental data show this down flow. It may be possible to reduce this deviation by fine-tuning some turbulence model parameter.

We have shown typical comparisons of the computed profiles of the three velocity components from the nonisotropic simulation results with the experimental data for three tank systems on the \( r-\theta \) and \( r-z \) planes. The validity of the calculated velocity field from the three-dimensional nonisotropic model was established by the comparison with the experimental data on 48 data points. The means of standard errors for the dimensionless radial, tangential and axial velocity components are 0.00229, 0.00033, and 0.00356, respectively. In next section, we will discuss the validation of the turbulence field.

4.2.2.2 Turbulence Field Validation

There are very limited experimental results for the turbulence intensities and turbulence energy dissipation rates. For our tank systems, the data of Patterson and Wu(28, Chapter II) is the only suitable for even a qualitative comparison. The turbulence field obtained from the nonisotropic model will be used for comparison because it described the experimentally measured velocity profiles.

The axial profiles of the nondimensional turbulence kinetic energy in the impeller stream are displayed in Figure IV-15. Two different radial positions were selected for each tank system to show typical results. The
Figure IV-15. Axial profiles of turbulence kinetic energy in different radial positions of impeller streams on 45° plane.
maximum in the turbulence kinetic energy occurs adjacent to the impeller tip. The turbulence kinetic energy diminishes quickly above and below the impeller stream. Also, it decreases with the radial direction. For the flow near the impeller, the turbulence kinetic energy is bigger than that near the horizontal faces of impeller blades, as shown by the profiles in Tank System 1. This reflects how jet has spread in the radial direction. However, as the radial distance is increased, the turbulence kinetic energy along the edge of the jet become as small as that of the flow in bulk regions. The turbulence kinetic energy profiles for Tank System 2 and Tank System 3 are comparable to those for Tank System 1.

The computed axial profiles of the dissipation rates of turbulence kinetic energy in the impeller jet are displayed in Figure IV-16. Two different radial positions were selected for each tank system. We find that the maximum dissipation rates are adjacent to the impeller tip, where the maximum turbulence kinetic energy occurs.

In Figure IV-16 we show two curves for the axial profiles of energy dissipation rates in Tank System 2 and Tank System 3, where the same impeller is used. These curves are for the same radial position but at different impeller speeds. We find two profiles of nondimensionalized dissipation rates merge to one in the bulk regions for the two radial positions shown. This implies that with same size of impellers, the normalized energy dissipation rates in the regions away from the jet are independent of the impeller speeds. Patterson and Wu(28, Chapter II) reported similar results based on experimental data as mentioned in the second chapter.

Patterson and Wu(28, Chapter II) measured turbulent intensity profiles through the impeller region which showed that the fluctuating components of the velocities in the impeller stream were higher than those in the
Figure IV-16. Axial profiles of turbulence energy dissipation rates in different radial positions of impeller streams on 45° plane.
bulk region. The turbulence kinetic energy is the sum of the square of
three velocity fluctuations, and the computed turbulence kinetic energy
profiles in Figure IV-15 show this same behavior. For the energy
dissipation rate, we were able to prepare a comparison of our computed
results with their experimental data in Figure IV-17. Both the simulation
results and the experimental data show that most of the turbulence energy
in an agitated vessel is dissipated in the impeller stream and both curves
have the same shape.

In the above discussion we showed that the turbulence field obtained
from the three-dimensional nonisotropic model qualitatively matches the
experimental results by Patterson and Wu (28, Chapter II). In the next
section, we will compare the performance of the three-dimensional
isotropic model with the nonisotropic model by showing solutions of the
governing equations with both of these models.

4.2.3 Comparison of Two Three-Dimensional Simulations

In Chapter III we proposed using two turbulence models for the flow in
agitated vessels. As discussed previously, the nonisotropic model
described the three-dimensional character of the turbulent flow in baffled
stirred tanks. The nonisotropic turbulence model is an extension of the
isotropic turbulence model incorporating the nonisotropic concept of
exchange coefficient $\Gamma$, and in this section a comparison is given for the
simulations using these two models.

In Figure IV-18, the dimensionless radial velocity profiles $V'$ along
the $\theta$-direction are compared for the simulations using the nonisotropic
and isotropic model at three values of $r$ and $z$ in the three tank systems.
Figure IV-18 is comparable to Figure IV-9 where the nonisotropic model was
Figure IV-17. Axial profiles of turbulence energy dissipation rates in Patterson and Wu's study (28, Chapter II) and in this work.
Figure IV-18. Radial velocity profiles along the $\theta$-direction obtained with two three-dimensional models.
compared with experimental data. As can be seen from the comparison of models in Figure IV-18, the velocity profiles for $V^1$ using the isotropic model were less than the velocity profiles with the nonisotropic model by as much as 50% in each of the three tank systems.

In Figure IV-19, the dimensionless tangential velocity profiles $W^1$ along the $\theta$-direction are compared at three values of $r$ and $z$ in three tank systems. In this case the velocity profiles for $W^1$ using the isotropic model were greater than those with the nonisotropic model by as much as 50% in each of the three tank systems. This shows that the nonisotropic turbulence model accounts for the effect of baffles by preventing the excessive rotation.

In Figure IV-20, the dimensionless axial velocity profiles $U^1$ along the $\theta$-direction are compared for the simulation using the nonisotropic and isotropic models at three values of $r$ and $z$ in the three tank systems. We find that the axial velocities with the isotropic model are lower than those from the nonisotropic model by 10% to 100% in the three tank systems.

A comparison of the profiles for the three velocity components along the $r$-direction obtained from the two three-dimensional simulations is given in Figures IV-21, IV-22, and IV-23 which are comparable to the comparisons of the velocity profiles with experimental data given in Figures IV-12, IV-13 and IV-14. These comparisons are generally similar to those for the $\theta$-profiles. The isotropic model predicted higher tangential velocities and smaller radial and axial velocities than the nonisotropic turbulence model. The three-dimensional nonisotropic $k-\varepsilon$ model is able to account for the baffling effects by reducing the rotation of fluid and by increasing the vertical flow. We conclude that the
Figure IV-19. Tangential velocity profiles along the θ-direction obtained with two three-dimensional models.
Figure IV-20. Axial velocity profiles along the θ-direction obtained with two three-dimensional models.
Figure IV-21. Radial velocity profiles along the r-direction on the 45° plane obtained with two three-dimensional models.
Figure IV-22. Tangential velocity profiles along the r-direction on the 45° plane obtained with two three-dimensional models.
Figure IV-23. Axial velocity profiles along the r-direction on the 45° plane obtained with two three-dimensional models.
isotropic turbulence model is not appropriate to describe the turbulent flow in baffled stirred tanks.

Before we leave this discussion of the three-dimensional simulations for the turbulent flow in agitated vessels, the CPU time of FPS-264 scientific computer used by the simulations with the two models should be discussed. In Table IV-2, the CPU time is given for both models in the three tank systems, and we can see that the nonisotropic simulation required about 1.7 times the CPU time than the isotropic model. This is because the nonisotropic model is more complicated than the isotropic model with those expressions related to the various viscosity components in the governing equations. The reason the three-dimensional simulation requires the amount of CPU time shown in the table is that a set of 92,736 or 81,144 algebraic equations are being solved iteratively for Tank System 1 or Tank Systems 2 and 3. Typically a solution requires about 650 iterations to converge from a good starting point provided by a two-dimensional simulation.

4.3 Two-Dimensional Simulation

The two-dimensional solutions of the governing equations neglect all the gradients of variables in the tangential direction. This reduces the number of independent variables by one, and it is an order of magnitude easier problem to solve as we have seen from the literature review and this work. However, omission of the \( \theta \) gradients does not describe the flow, but these solutions can serve as an approximation to the flowfield. As we mentioned earlier, the three-dimensional models were developed from the corresponding two-dimensional models. Our approach was to derive the differential and discretized governing equations and develop a computer
Table IV-2. CPU Time in Minutes on FPS-264 for Two Three-Dimensional Simulations.

<table>
<thead>
<tr>
<th>Tank System</th>
<th>Isotropic Model</th>
<th>Nonisotropic Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>121.03</td>
<td>223.07</td>
</tr>
<tr>
<td>2</td>
<td>94.27</td>
<td>153.07</td>
</tr>
<tr>
<td>3</td>
<td>101.62</td>
<td>170.72</td>
</tr>
</tbody>
</table>
code for the three-dimensional flow. We used the two-dimensional numerical results for the initial estimates of the variables in the three-dimensional computations in order to reach converged solutions with less computer time.

The two-dimensional simulation for the turbulent flowfield in agitated vessels has its own value for some applications such as fermentation(1) where the flow in the jet zone is important for microbiological reasons. As we discussed in the preceding section of this chapter, it happens that the flow in this part of the stirred tanks is dominated by the rotating impeller, and the tangential gradients are negligible there. For such applications, two-dimensional simulation may be more practical than three-dimensional simulation because of the significantly reduced computer time and efforts. Recently, Robertson and Ulbrecht(1) measured the shear rates in the region near impellers for numerous combinations of impeller diameters and rotating speeds in laboratory scale fermenters using a platinum wire as the working electrode. They used the measured shear rates to obtain a maximum-shear-rate correlation for the purpose of scale-up. They claimed a difficulty to have accurate measurement caused by the ion concentration and diffusivity(1). Also, Mulvahill(6, Chapter I) could not measure the velocity profiles in this region because the wire of hot wire anemometer would break.

Without the difficulty encountered in experiments, numerical simulation of the flow can provide the flow patterns not only for lab-scale but even for plant-scale reactors. As a result, it is worthwhile to obtain the simulation results from two-dimensional models. Computer time and storage used in two-dimensional calculations are much less than those required for three-dimensional computations, and we can afford to compare the performance of more turbulence models in two-dimensional than in
three-dimensional simulations. In this research, four two-dimensional models are compared, and the details of these four two-dimensional simulations will be given.

4.3.1 Consideration of Drag Effects

Results from the two-dimensional simulation with the standard k-ε model did not fit the experimental data. It predicted higher values of the tangential velocity than the experimental data. Harvey and Greaves (6, Chapter II) recognized this problem and added a drag term in the angular momentum equation. The effect was to reduce the tangential velocity, and simulate the baffling effects artificially. In this research we proposed a drag term in the jet zone and another one for the flow in the recirculation region, since the flows in these two areas are very different. These drag terms were expressed in equations (III-42a,42b) where two drag coefficients were determined by comparison with measured velocity profiles.

Figures IV-24 and IV-25 show how the calculated velocity profiles in the bulk region and jet zone of Tank System 1 are changed by adding the two drag terms in the angular momentum equation to account for the baffling effects. The radial and axial velocities are only slightly changed, either increased or decreased. This is because they are affected only indirectly by the drag term in the angular momentum equation. For the tangential velocity $W_1$ in the bulk region, there is a significantly decrease near the tank wall, but there is an increase in those places away from the wall. In the discharge flow region, however, the tangential velocity from the model with the drag term is less than the corresponding velocity from the model without the drag term. From Figure B-13 to B-16,
Figure IV-24. The drag effects on velocity in the bulk region of Tank System 1. The number on the left in parenthesis is $C_{Drj}$, and the one on the right is $C_{Drb}$. 
Figure IV-25. The drag effects on velocity in the jet zone of Tank System 1. The number on the left in parenthesis is $C_{Drj}$, and the one on the right is $C_{Drb}$. 
we also find the drag term in the angular momentum equation causes similar changes of velocity in both jet zones and bulk regions of Tank System 2 as well as Tank System 3. The justification for adding the drag terms to describe the baffling effects is based on obtaining a better fit to experimental data.

The two drag coefficients $C_{Drj}$ and $C_{Drb}$ of Equations (III-42a, 42b) have to be determined by comparing numerical tangential velocity profiles with those from experimental data. After trying numerous pairs of $C_{Drj}$ and $C_{Drb}$, we found that there was a good fit for the tangential velocity in both the recirculation zone and discharge stream for all three tank systems when $C_{Drj}$ ranged between $1/200$ and $1/300$ and $C_{Drb}$ between $1.0$ and $2.0$. However, no optimal pair for $(C_{Drj}, C_{Drb})$ was found.

A typical example is given in Figure IV-26 which shows the computed tangential velocity component fits the tangential jet with the five pairs of drag coefficients listed on the figure for all three tank systems. However, for the bulk region none of five tangential velocity profiles fit the experimental data, as shown in Figure IV-27 for the three tank systems. Some pairs are closer to the experimental data than others. For example, the tangential velocity profiles associated with the pair $(1/250, 2.0)$ in the bulk region of Tank System 1 is closest to the data; In Tank System 3, however, this pair of drag coefficients leads to worst match among the five pairs of coefficients. Faced with this situation, we decided to use the values in the middle of the ranges for $C_{Drj}$ and $C_{Drb}$, i.e.,

\[
C_{Drj} = 1/250
\]

\[
C_{Drb} = 1.5
\]

in the two-dimensional isotropic model proposed in this research.
Figure IV-26. The tangential velocity component in the jet zone for three tank systems with five pairs of drag coefficients.
Figure IV-27. The tangential velocity in the bulk region of three tank systems with five pairs of drag coefficients.
4.3.2 Comparison of Four Two-Dimensional Simulations

In previous subsection, we have determined the two drag coefficients to complete our two-dimensional isotropic model. We can now compare the performance among the four different two-dimensional turbulence models which are given in Table IV-3. Model 1 is the isotropic turbulence model and Model 2 is the nonisotropic turbulence model used in this work. These two models incorporated the swirling effects and baffling effects. Model 3 is the one used by Harvey and Greaves(6, Chapter II) which did not include the swirling effects. Model 4 is the standard k-ε turbulence model used by Middleton, et al.(5, Chapter I) which did not include the swirling effects and baffling effects. However, Middleton, et al.(5, Chapter I) reported a three-dimensional simulation with this model. As listed in Table IV-3, model coefficients are different for these four models.

The radial velocity profiles from the impeller tip to the tank wall are displayed in Figure IV-28 at three axial positions for the four simulations and the tangential jet. These profiles give typical results in the jet zone; and they are 0.25" above the 3"-impeller plane in Tank System 1, 0.15" above the 4"-impeller plane in Tank System 2, and 0.05" above the 4"-impeller plane in Tank System 3. The radial velocity profiles for all four turbulence models have the same shape but underpredict the tangential jet in all tank systems. The deviation between the numerical and analytical radial velocity profiles increase with increasing radial distance. The deviation near the wall may be explained partially by the fact that the tangential jet does not describe the flow in this region.

Among the four numerical radial velocity profiles, the nonisotropic k-ε model (Model 2) matches the tangential jet better than three other
Table IV-3. Differences of Four Versions of Two-Dimensional \(k\)-\(\varepsilon\) Turbulence Model.

<table>
<thead>
<tr>
<th>Isotropy</th>
<th>Swirling effects</th>
<th>Baffling effects</th>
<th>Model Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model 1(^*)</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>(C_\mu)</td>
<td>eqn (III-34)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_1)</td>
<td>eqn (III-35)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_2)</td>
<td>eqn (III-36)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_k)</td>
<td>0.87</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_\varepsilon)</td>
<td>1.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model 2(^*)</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>(C_\mu)</td>
<td>eqn (III-34)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_1)</td>
<td>eqn (III-35)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_2)</td>
<td>eqn (III-36)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_k)</td>
<td>0.87</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_\varepsilon)</td>
<td>1.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model 3(^*)</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>(C_\mu)</td>
<td>0.09</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_1)</td>
<td>1.43</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_2)</td>
<td>1.92</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_k)</td>
<td>0.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_\varepsilon)</td>
<td>0.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Model 4(^*)</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>(C_\mu)</td>
<td>0.09</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_1)</td>
<td>1.44</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_2)</td>
<td>1.92</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_k)</td>
<td>1.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_\varepsilon)</td>
<td>1.3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(^*\): The isotropic \(k\)-\(\varepsilon\) model proposed in this study.

\(^\dagger\): The nonisotropic \(k\)-\(\varepsilon\) model proposed in this study.

\(^\ddagger\): The modified \(k\)-\(\varepsilon\) model by Harvey and Greaves(6, Chapter II).

\(^\ddagger\ddagger\): The classic \(k\)-\(\varepsilon\) model by Launder and Spalding(4, Chapter III).

*: In Model 1 and 3, the baffling effects are accounted for by adding drag terms in the angular momentum equation. In model 2, effects are considered through the nonisotropic viscosity coefficient.
Figure IV-28. Radial velocity at three different axial positions in the discharge stream of three tank systems.
isotropic k-ε models in different tank systems. Model 3, used by Harvey and Greaves (6, Chapter II), does as poorly as Model 4, i.e. the classic k-ε turbulence model. This means the slight changes in model coefficients, as shown in Table IV-3, and the inclusion of their drag term to account for the baffling effects failed to enhance the accuracy of the radial velocity components in the discharge stream. On the other hand, Model 1, which incorporated the swirling effects and baffling effects, provided a better fit for radial velocity profiles than Model 3, especially in Tank System 2 and Tank System 3, where 4" impeller is used.

The radial velocity profiles in the bulk regions of three tank systems are displayed in Figure IV-29. Again, three different axial positions are selected to show typical results from the comparisons between predicted velocity profiles and experimental data. The three axial positions are 4.5" above, 3.75" above, and 2.25" above the impeller plane of Tank System 1, Tank System 2, and Tank System 3, respectively. Among the four predicted velocity profiles, the one from Model 4 has a different shape than three others in Tank System 1 and Tank System 2. The other three profiles have same shapes in all three tank systems. In Tank System 1, we find the radial velocity profiles obtained from Model 1 and Model 2 fit the measured data reasonably well. In Tank System 2, the radial velocity profiles of Model 1 and Model 2 were closer to the experimental data than the other two models. As for the radial velocity profiles in Tank System 3, the four models had the same shape, but none of them fit the experimental data very well.

The profiles of tangential velocity W' in the jet zones of three tank systems are plotted for three axial positions in Figure IV-30. This figure shows that Model 4 overestimates the tangential velocity significantly in all cases. The profiles for Model 1 and Model 3 provide
Figure IV-29. Radial velocity at three different axial positions in the bulk regions of three tank systems.
Figure IV-30. Tangential velocity at three different axial positions in the discharge stream of three tank systems.
a good match to the analytical tangential velocity profiles for various tank systems, even though both models slightly overestimate the tangential velocity in the jet stream of Tank System 1 and underestimate them in Tank System 3. Both of these models have drag terms to account for the baffling effects. Model 1 gives a more accurate prediction of the tangential velocity in the jet zone of Tank System 3, but neither model is superior to the other one. Model 2, the nonisotropic k-ε model, is much better than the standard k-ε model, but still overestimates the tangential velocity in the jet zone. Its prediction of the tangential velocity in the jet zone is worse than the isotropic turbulence models with modifications made for the angular momentum equation by adding drag terms. This is because the reduction of tangential velocity was made indirectly through the anisotropy in Model 2, while Model 1 and Model 3 purposely reduce the velocity through the angular momentum equation.

Figure IV-31 displays the tangential velocity profiles in the bulk regions of agitated vessels. Like in the impeller stream, the standard k-ε model significantly overpredict the tangential velocity. The other three models fit the measured profiles relatively well. All of the three models do equally well. Model 1 and Model 3 perform better in the places away from tank wall, but Model 2 has better match with experimental data near the tank wall.

For the axial velocity profiles in the jet zone shown in Figure IV-32, the standard k-ε model in the three tank systems have a different shape than the tangential jet. The other three modified versions of k-ε model have same shape profile of the axial velocity from the tangential jet. These three models, however, underestimate the axial velocity away from the tank wall in all tank systems. In the positions 0.25" above the impeller plane of Tank System 1 and 0.15" above the impeller plane of Tank
Figure IV-31. Tangential velocity at three different axial positions in the bulk regions of three tank systems.
Figure IV-32. Axial velocity at three different axial positions in the discharge stream of three tank systems.
System 2, the axial velocity obtained from the nonisotropic $k$-$\varepsilon$ model, i.e. Model 2, matched the analytical axial velocity profiles better than those from isotropic Model 1. Also, Model 1 performed better than Model 3, which is used by Harvey and Greaves (6, Chapter I). In Tank System 3, the axial velocity profiles from Model 1 to Model 3 are basically the same.

Figure IV-33 displays the axial velocity profiles at three different positions in the bulk regions of three tank systems. Once again, Model 4 behaves differently than the other three models, and all underestimate the axial velocity. In the region away from the tank wall of Tank System 1, the axial velocity profiles predicted by Model 3 are closer to the experimental data than Model 1 and Model 2. Near tank wall, however, Model 1 and Model 2 perform better than Model 3. The same results are observed in Tank System 2 and Tank System 3. From Figure IV-33, we also find the axial velocity profiles predicted by Model 1 and Model 2 are very close, especially near the tank wall.

In summary, we have presented comparisons among the different velocity profiles at different locations in the different tank systems for the four different two-dimensional models. We conclude that the standard $k$-$\varepsilon$ model is not suitable to describe the turbulent flow in impeller-driven baffled agitated vessels. Modification of this turbulence model is required, and this was done in Model 1 and Model 3 by changing the model coefficients and adding drag terms in the angular momentum equations to purposely reduce the tangential velocity. These two models gave a better fit to the data. From Figure IV-28 to IV-33, we find generally Model 1 is a slightly better than Model 3. Model 1 considered the swirling effects and the drag terms associated with this model are more elaborate. However, Model 2, the nonisotropic turbulence model, had the best agreement with the
Figure IV-33. Axial velocity at three different axial positions in the bulk regions of three tank systems.
experimental data. Among the velocity profiles shown in Figure IV-28 to IV-33, only the tangential velocity in the impeller stream obtained from the nonisotropic turbulence model deviated further from the tangential jet than those obtained from the other two modified isotropic turbulence models, i.e. Model 1 and Model 3. Other than that, the nonisotropic k-ε model perform better or at least as good as its isotropic counterparts. This is to be expected, because the model is more realistic for describing the swirling character of the flowfield in agitated vessels. Also, Model 2 in three-dimensional simulation matched the experimental data much better than Model 1. In the two-dimensional analysis, the capability to describe the flow patterns by Model 1, after modified with drag terms, is close to Model 2.

The comparison of different models is not complete until their CPU time, listed in Table IV-4, is considered. It is no surprise that the two-dimensional nonisotropic model required more CPU time than the isotropic models, and this was the same for the three-dimensional simulation. The CPU time for the two dimensional simulations ranged from 3.13 to 7.42 minutes on the IBM 3084, and the CPU time for the three-dimensional simulations ranged from 94.27 to 223.07 minutes on the FPS-264 scientific computer.

4.4 Comparison of Previous Studies

The best way to evaluate the performance of different turbulence models is to use them in the same system to obtain numerical results and compare these results with experimental data. In previous sections, we have made comprehensive comparisons quantitatively among different turbulence models. Some of them were used by other investigators to describe the
Table IV-4. CPU Time in Minutes on IBM 3084 for Four Two-Dimensional Simulations.

<table>
<thead>
<tr>
<th>Model</th>
<th>Tank System 1</th>
<th>Tank System 2</th>
<th>Tank System 3</th>
<th>Model Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.35</td>
<td>3.37</td>
<td>3.13</td>
<td>Isotropic, Swirling, Baffling</td>
</tr>
<tr>
<td>2</td>
<td>7.42</td>
<td>5.65</td>
<td>6.02</td>
<td>Nonisotropic, Swirling, Baffling</td>
</tr>
<tr>
<td>3</td>
<td>4.13</td>
<td>3.65</td>
<td>3.62</td>
<td>Isotropic, Baffling</td>
</tr>
<tr>
<td>4</td>
<td>4.30</td>
<td>3.78</td>
<td>3.97</td>
<td>Isotropic</td>
</tr>
</tbody>
</table>
turbulent flow in agitated vessels. The result of these comparisons was that the nonisotropic k-ε turbulence model is superior to other isotropic k-ε models for the turbulent flowfield in agitated vessels. However, the turbulence model is only part of the numerical simulation for the turbulent flowfield, as indicated in Chapter III. Other elements in the simulation such as boundary conditions and numerical method are also important. In this section, we will compare our simulation with the other studies on the turbulent flow in agitated vessels. Through these comparisons, we will establish how this research compares with other works and show our contribution to extend the description of the turbulent flow in agitated vessels.

4.4.1 Three-Dimensional Simulations

The work by Middleton, et al. (5, Chapter I) is the only three-dimensional study on the flowfield of agitated vessels in the literature. Table IV-5 listed the comparison of their study and this research as to the following important aspects of simulation: turbulence model, boundary conditions at the turbine blades, material balance of the blade-swept region, numerical technique, and the validation of velocity and turbulence fields.

The Navier-Stokes equations were used in both studies, but the closure models were different. Middleton, et al. (5, Chapter I) used the standard k-ε turbulence model which does not consider the effects of rotation. In this research, we used two k-ε models. One is the isotropic turbulence model, which is directly modified from the standard k-ε model by adding the rotational effects. The other is the nonisotropic turbulence model which allows for six different viscosity components and is a flexible
Table IV-5. Comparison of the Three-Dimensional Simulations for the Turbulent Flow in Agitated Vessels for Middleton, et al. (5, Chapter I) and This Research.

<table>
<thead>
<tr>
<th></th>
<th>Middleton, et al.</th>
<th>This research</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbulence model</td>
<td>Standard isotropic two-equation model</td>
<td>Modified isotropic and nonisotropic two-equation models</td>
</tr>
<tr>
<td>B.C. at impeller blades</td>
<td>Laser velocimeter measurement</td>
<td>Zero-gradient assumptions &amp; tangential jet</td>
</tr>
<tr>
<td>Material balance in blade region</td>
<td>Not reported</td>
<td>Outflow required to match inflow</td>
</tr>
<tr>
<td>Numerical method</td>
<td>Finite domain method</td>
<td>Finite domain method</td>
</tr>
<tr>
<td>Velocity field validation</td>
<td>Not reported</td>
<td>Comparison with experimental data for three velocity components</td>
</tr>
<tr>
<td>Turbulence field validation</td>
<td>Not reported</td>
<td>Qualitative comparison with experimental data in the impeller stream</td>
</tr>
</tbody>
</table>
extension of the isotropic turbulence model. Through these components, we were able to describe accurately the turbulent flowfield of agitated vessels by highlighting the swirling jet from the rotational impellers and the baffling effects of the flow patterns.

The values of variables at the turbine blade periphery are needed as boundary conditions for the solution of conservation equations. Middleton, et al. (5, Chapter I) reported that these variables were measured by the laser anemometer. In this research, we used the values obtained from the tangential jet as the boundary conditions for the three velocity components at the impeller tip. Zero-gradient assumptions for turbulence parameters at the impeller tip were made. Assumptions such as zero-gradient of variables were also made to provide the other boundary conditions. Also, the material balance in this region must be maintained. Middleton, et al. (5, Chapter I) did not report that the material balance has been considered when they specified the boundary conditions for the variables in the blade-swept region. In this research, the material balance is required to be satisfied.

The numerical technique used in both studies is the same, i.e. the finite domain method. The only calculated results for the flowfield reported by Middleton, et al. (5, Chapter I) were shown in Figure II-1, and no comparison with experimental data was reported to validate their solution. In this research, we used Mulvahill's (6, Chapter I) velocity measurements for quantitative comparisons and Patterson and Wu's (28, Chapter II) data of turbulence intensities and energy dissipation rates in the impeller stream for qualitative comparisons. It was not feasible to make a direct comparison between these two three-dimensional simulation studies, but there is qualitative agreement in the shape of velocity
vectors as shown by examining Figures IV-1 and IV-2 for this research and Figure II-1 for the study of Middleton, et al. (5, Chapter I).

4.4.2 Two-Dimensional Simulations

Even though the flow in agitated vessels are three-dimensional, the two-dimensional axisymmetrical simulations have been used because the governing equations are easier to solve. Table IV-6 illustrates the details of different two-dimensional simulations for the turbulent flow in agitated vessels.

As shown in Table IV-6, the turbulence models used in these two-dimensional simulations are different. Some of the details about these turbulence models were provided in previous chapters and were summarized in Table IV-3. In this research we used all these turbulence models except the isotropic three-equation turbulence model by Placek, et al. (12, Chapter II). This three-equation turbulence model had two transport equations for the turbulent kinetic energy as shown in Chapter II.

Platzer (11, Chapter II) and Placek, et al. (12, Chapter II) did not consider the baffling effects in their numerical simulation. Harvey and Greaves (10, Chapter II) used a drag term for this purpose. In our research, we used drag terms in the isotropic model and the different viscosity components in the nonisotropic model to account for the baffling effects.

As discussed in the previous subsection, the boundary conditions on the periphery of the impeller blades are required. Harvey and Greaves (10, Chapter II) made assumptions such as zero-gradient to provide the necessary boundary conditions. In this research and Platzer's work (11,
Table IV-6. Comparison of the Two-Dimensional Simulations for the Turbulent Flow in Agitated Vessels for Platzer (11, Chapter II), Placek, et al. (12, Chapter II), Harvey and Greaves (10, Chapter II), and this research.

<table>
<thead>
<tr>
<th></th>
<th>Platzer</th>
<th>Placek, et al.</th>
<th>Harvey and Greaves</th>
<th>This research</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbulence model</td>
<td>Standard isotropic two-equation</td>
<td>Modified isotropic three-equation</td>
<td>Modified isotropic two-equation</td>
<td>Modified isotropic &amp; nonisotropic two-equation models</td>
</tr>
<tr>
<td></td>
<td>model</td>
<td>model</td>
<td>model</td>
<td>models</td>
</tr>
<tr>
<td>Baffling effects</td>
<td>Not considered</td>
<td>Not considered</td>
<td>Considered with a drag term</td>
<td>Considered with drag terms and nonisotropy</td>
</tr>
<tr>
<td>B.C. at impeller blades</td>
<td>Zero-gradient assumptions &amp; tangential jet</td>
<td>Zero-gradient assumptions &amp; trailing vortex model</td>
<td>Assumptions (e.g. zero-grad) &amp; tangential jet</td>
<td>Zero-gradient assumptions &amp; tangential jet</td>
</tr>
<tr>
<td>Numerical method</td>
<td>Stream function and vorticity transformations</td>
<td>Stream function and vorticity transformations</td>
<td>Finite domain method</td>
<td>Finite domain method</td>
</tr>
<tr>
<td>Velocity field validation</td>
<td>For three velocity components</td>
<td>For the resultant velocity components</td>
<td>For three velocity components</td>
<td>For three velocity components</td>
</tr>
<tr>
<td>Turbulence field validation</td>
<td>Qualitative &amp; partly quantitative</td>
<td>Qualitative</td>
<td>Qualitative</td>
<td>Qualitative</td>
</tr>
</tbody>
</table>
Chapter II) the tangential jet model was used to obtain values at the impeller tip. However, Placek, et al. (12, Chapter II) used the complicated implicit trailing vortex model. When the boundary conditions are specified for the impeller periphery, the material balance over the blade-swept region must be satisfied. However, the previous studies did not report how the material balance was satisfied.

Two numerical techniques were used to solve conservation equations. They were the stream function and vorticity transformations used by Platzer (11, Chapter II) and Placek, et al. (12, Chapter II) and the finite domain method used by Harvey and Greaves (10, Chapter II) and this study. The stream function and vorticity transformations eliminate the calculation for pressure field, but this method cannot be extended to three-dimensional flowfields. The finite domain method needs to solve for the pressure field, but it is straightforward to extend the solution procedure from two-dimensional to three-dimensional as we have done in this research.

All of these four two-dimensional simulation studies had comparisons of computed results and experimental data. The velocity field validation made by Placek, et al. (12, Chapter II) was for the resultant velocity. In the other three studies, the validation of velocity field was made through the comparisons for the three velocity components. As for the turbulence field validation, qualitative comparisons were made in all studies. Platzer (11, Chapter II) made the only quantitative comparison for the turbulence kinetic energy in the bulk region with his data which showed qualitative agreement.

It was not feasible to make a conclusion that some two-dimensional simulation is superior to the others, since the two-dimensional simulation inherently lead to the discrepancies between experimental data and
computed results due to the omission of the $\theta$-gradients. However, from the above comparisons for different two-dimensional simulations, we still can make some suggestions for a good two-dimensional approximate study for the flowfield in agitated vessels in the future. First, the nonisotropic model or the isotropic model with the drag terms to account for the baffling effects should be used. Also, the boundary conditions at the turbine periphery must be carefully specified so that the material balance would be satisfied. In addition, the flexible finite domain method is a better choice than the stream function and vorticity transformations. Finally, the simulation studies require more experimental data, especially turbulence kinetic energy and dissipation rate, for the validation purpose.

4.5 Convergence and Accuracy

The convergence of the numerical solution is measured by how well the continuity equation is satisfied as discussed in Chapter III. The accuracy of the numerical solution is measured by how well results compare at the same grid point for different size grids. The accuracy of the simulation is measured by how well the solution compares with experimental data. The first comparison establishes the accuracy of the numerical solution. Comparison with experimental data establishes that the numerical solution of the conservation equations describes the flow phenomena in the stirred tank.

When the transport equations were discretized, the continuity equation became a source term in the pressure-correction equation in the SIMPLE and SIMPLER algorithms. Both algorithms required this source term to be zero as the criterion for convergence. The residual of the continuity equation
had to be less than a small number for convergence to be reached. $10^{-15}$ was used for entire calculation domain, and $10^{-4}$ was used for each finite subdomain. Additional criteria of convergence were also used and residuals of other transport equations, i.e. the momentum equations, k-equation and $\varepsilon$-equation, were required to be less than small numbers. For any finite domain, $10^{-6}$ was used for the momentum equations and $10^{-5}$ was used for the k- and $\varepsilon$-equation. The relative change from iteration to iteration of the variables on any grid point were required to be smaller than $10^{-4}$.

The convergence to a solution depended on the initial estimates for variables. Zero was used for all three velocity components in the two-dimensional computations. SIMPLE algorithm required an initial estimate for pressure field, and the sum of atmospheric pressure and static pressure was used in the two-dimensional simulations. An initial estimate for the turbulence field was also required. The turbulent viscosity was calculated from equations (III-25) and (III-50) which contain both k and $\varepsilon$. Estimates for these two variables which were not sufficiently close to the actual values may lead to divergence. Thus, a procedure was developed to obtain an estimate for k and $\varepsilon$ which was related to the impeller speed and diameter since the turbulent flow is driven by the impeller. From a simple dimensional analysis, the following expression for k was developed in terms of two impeller parameters, i.e. N and $D_{i}$.

$$k = N^2D_{i}^2$$

where N and $D_{i}$ are the rotating speed and diameter of the impeller in SI unit. Using the same parameters, we can obtain the following expression for $\varepsilon$: 

The proportional constants were obtained by numerical experimentations, and the values calculated from the following two equations were used as initial estimate for $k$ and $\varepsilon$ for the two-dimensional models in the three tank systems.

\[ k = 0.16 \, N^2 D_i^2 \]

\[ \varepsilon = 0.32 \, N^2 D_i^2 \]

For the three-dimensional solution, the computed results from the two-dimensional models were used as the initial estimates. The estimates using the two-dimensional numerical results were closer to the actual flowfield solution and were able to provide faster convergence for the expensive three-dimensional calculations.

To help avoid divergence, relaxation factors were utilized with the iteration technique. We had to slow down the changes in values of dependent variables from iteration to iteration by using the relaxation factors. In Tables IV-7 and IV-8 the typical relaxation factors used in different models are listed. These numbers were different for different models, but they applied to all three tank systems. It should be pointed out that the relaxation factors listed in Tables IV-7 and IV-8 were obtained from extensive exploratory numerical experimentations. They guaranteed the convergence for the flowfield in all three tank systems here, but this does not mean that they are the optimal values. Some of them were constant to the end of the iterations, and the others could increase during the iterating process in order to have quicker convergence. Also, no rules were developed to make those changes to the relaxation factors. The relaxation factor for the variable $P$ was 1.0 for
Table IV-7. Relaxation Factors in Four Two-Dimensional Simulations of the Turbulent Flow in Three Stirred Tank Systems.

<table>
<thead>
<tr>
<th>Model</th>
<th>$\beta_V$</th>
<th>$\beta_{rW}$</th>
<th>$\beta_U$</th>
<th>$\beta_P$</th>
<th>$\beta_K$</th>
<th>$\beta_\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.35$^+$</td>
<td>0.35$^+$</td>
<td>0.40$^+$</td>
<td>0.5</td>
<td>0.40$^+$</td>
<td>0.40$^+$</td>
</tr>
<tr>
<td>2</td>
<td>0.50</td>
<td>0.50</td>
<td>0.50</td>
<td>0.5</td>
<td>0.60</td>
<td>0.60</td>
</tr>
<tr>
<td>3</td>
<td>0.35$^+$</td>
<td>0.35$^+$</td>
<td>0.40$^+$</td>
<td>0.4</td>
<td>0.40</td>
<td>0.40</td>
</tr>
<tr>
<td>4</td>
<td>0.40$^+$</td>
<td>0.60$^+$</td>
<td>0.50$^+$</td>
<td>0.4</td>
<td>0.40</td>
<td>0.40</td>
</tr>
</tbody>
</table>

$^+$: These relaxation factors are subject to increase by 0.05 for every 40 iterations until a maximum of 0.9 is reached.

$^\mathbb{R}$: These numbers are used in the SIMPLE algorithm, and they are replaced by 1.0 in the SIMPLER algorithm.

---

Table IV-8. Relaxation Factors in Two Three-Dimensional Simulations of the Turbulent Flow in Three Stirred Tank Systems.

<table>
<thead>
<tr>
<th>Model</th>
<th>$\beta_V$</th>
<th>$\beta_{rW}$</th>
<th>$\beta_U$</th>
<th>$\beta_P$</th>
<th>$\beta_K$</th>
<th>$\beta_\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>0.35$^+$</td>
<td>0.45$^+$</td>
<td>0.40$^+$</td>
<td>0.5</td>
<td>0.40</td>
<td>0.40</td>
</tr>
<tr>
<td>Nonisotropic</td>
<td>0.30</td>
<td>0.30</td>
<td>0.35</td>
<td>0.5</td>
<td>0.30</td>
<td>0.30</td>
</tr>
</tbody>
</table>

$^+$: These relaxation factors are subject to increase by 0.05 for every 40 iterations until a maximum of 0.9 is reached.
the pressure equation in the SIMPLER algorithm. However, it was 0.4 to
0.5 when applied to the following equation \( P = P^* + \beta P' \) to reduce the
exaggerated pressure correction made by \( P = P^* + P' \) in the SIMPLE algorithm
as shown in Table IV-7.

The linearization of the source terms also played an important role in
convergence. Linearization of the source terms may have the same effect
as providing relaxation factors. This can be seen by comparing the
coefficient \( C_p \) before and after the linear treatment of the source terms,
i.e. equations (III-78e, 78g). This helped to converge the iterations by
slowing down the changes in the variables during iterations. To have
strong under-relaxation, we linearized the source term as:

\[
S_\phi = (S_{\phi_1} + A \phi P^*) + (S_{\phi_2} - A) \phi P
\]

where \( A \) stands for positive numbers greater than 1.

This linearization scheme was particularly useful when large source
terms made undesirably large changes in the variables. All of the source
terms for different variables were placed in the subroutine SOURCE in the
computer program in Appendix C.

In addition to convergence, the accuracy of the numerical calculation
also needed to be established. When the number of the grid points
approaches infinity, the solution of the discretized equations usually
approaches the solution of the differential equations. However, it is not
computationally feasible to have an unlimited number of grid points.
Consequently, a check for accuracy is usually made by varying the number
of grid points in the calculation domain and comparing the values of the
dependent variables at the same grid points. The goal is to reduce the
computer storage and execution time by choosing a grid size with a
smallest number of grid points which provide the accuracy to an acceptable degree.

Figure IV-34 shows a comparison of three nondimensional velocity components from the two-dimensional solution at four different mesh sizes. The profiles are in the axial position of 4.5 inches above the 3-inch impeller plane. The four curves indicate that the calculated results corresponding to the mesh size 26x30 in the r-z plane are close to those associated with the larger mesh sizes 30x35 and 36x40, but there are discrepancies in the smaller 16x20 mesh. Table IV-9 shows the three velocity components at the same grid point with four grids for the two-dimensional solution with SIMPLE algorithm. It indicates that the values obtained from the grids 26x30, 30x35 and 36x40 agreed within one to two significant figures. Comparable results were obtained at other grid points; and thus, we selected the 26x30 mesh for the calculation domain in the r-z plane of the tank with the 3-inch impeller.

For the three-dimensional solution the size of the distance along the tangential direction was about 4/5 of the axial distance in the calculation domain, and the number of grid points in the θ-direction was set to be 25 to give a grid of 26x30x25 grid. A different variable spacing was needed for the tank with the 4-inch impeller and a mesh size of 23x30x25 was used. The grid spacing was given in the sample output in Appendix D.

It was not possible to do a convergence and accuracy study for the three-dimensional solution because of the computer storage and CPU time required. As was shown in Table IV-2 a three-dimensional solution required 163 to 223 minutes of CPU time on the FPS-264 advanced processor with the mesh sizes we used in this study. It was not feasible to select one of the larger grids in the two-dimensional solution because of
Figure IV-34. Accuracy checked by comparing the computed velocity profiles corresponding to four different meshes.
Table IV-9. Nondimensional Velocity Components at $r'=3.46$ and $z'=3.0$ in Tank System 1 with Various Grids.

<table>
<thead>
<tr>
<th>Mesh Size</th>
<th>$V'$</th>
<th>$W'$</th>
<th>$U'$</th>
<th>CPU time on IBM 4341</th>
</tr>
</thead>
<tbody>
<tr>
<td>16x20</td>
<td>-0.0321</td>
<td>0.0583</td>
<td>0.0488</td>
<td>21.22 min.</td>
</tr>
<tr>
<td>26x30</td>
<td>-0.0139</td>
<td>0.0381</td>
<td>0.0194</td>
<td>33.62 min.</td>
</tr>
<tr>
<td>30x35</td>
<td>-0.0116</td>
<td>0.0380</td>
<td>0.0158</td>
<td>40.47 min.</td>
</tr>
<tr>
<td>36x40</td>
<td>-0.0102</td>
<td>0.0368</td>
<td>0.0109</td>
<td>51.23 min.</td>
</tr>
</tbody>
</table>
computer storage and time as shown on Table IV-9 when CPU time was from 33 to 51 minutes on IBM 4341.

4.6 Algorithm Comparison

A solution procedure had to be selected which used either the SIMPLE or the SIMPLER algorithm to solve two-dimensional nonlinear governing equations. Both algorithms were able to solve the equations and the one to be selected would use the least amount of CPU time. This same algorithm would be used in time-consuming three-dimensional calculations.

Both algorithms were used to solve the governing equations with the isotropic k-ε model for the flow in the tank with the 3" impeller at 250 rpm (Tank System 1) and with the nonisotropic k-ε model for the flow in the tank with the 4" impeller at 150 rpm (Tank System 2). All other conditions for the calculations such as criteria of convergence and mesh sizes were the same except that the relaxation factors $\beta_p$ were different, as shown in Table IV-7.

Figures IV-35 and IV-36 compare typical results using the two algorithms, and essentially the same results are obtained with both algorithms for the velocity components, turbulence energy, and dissipation rate. This can provide the convergence, accuracy and validity for each algorithm and the only difference was computer time for a solution.

The comparison of CPU time on IBM 4341 and FPS-264 is shown in Table IV-10 for the SIMPLE and SIMPLER algorithm. This shows that the SIMPLE algorithm required less CPU time for convergence than the SIMPLER algorithm for the turbulent flow in both Tank Systems 1 and 2 with the isotropic and nonisotropic k-ε models. This was probably caused by the fact that the SIMPLER algorithm had to solve one more equation, i.e. the
Figure IV-35. Nondimensional velocity profiles computed with the SIMPLE and SIMPLER algorithm in the two-dimensional simulation of the turbulent flow in Tank System 1.
Figure IV-36. Profiles for $k'$ and $\varepsilon'$ computed with the SIMPLE and SIMPLER algorithm in the two-dimensional simulation of the turbulent flow in Tank System 2.
Table IV-10. CPU Time for the SIMPLE and SIMPLER Algorithms.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>CPU time on IBM 4341</th>
<th>CPU time on FPS-264</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tank System 1, Isotropic Model</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SIMPLE</td>
<td>33.62 min.</td>
<td>2.20 min.</td>
</tr>
<tr>
<td>SIMPLER</td>
<td>53.32 min.</td>
<td>8.55 min.</td>
</tr>
<tr>
<td>Tank System 2, Nonisotropic Model</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SIMPLE</td>
<td>59.23 min.</td>
<td>3.93 min.</td>
</tr>
<tr>
<td>SIMPLER</td>
<td>95.30 min.</td>
<td>15.10 min.</td>
</tr>
</tbody>
</table>
pressure equation, in every iteration. To have quicker convergence the SIMPLER algorithm must save more time than the additional time spent on solving this extra equation. Also, the three-dimensional calculations had to be performed on the FPS-264 scientific computer, and the SIMPLER algorithm had an inherent disadvantage with the FPS machine. The SIMPLER algorithm requires more input-output processing, but the FPS machine counts the IO time in the CPU time. As shown in Table IV-10, SIMPLER consumed about 1.6 times the CPU time as SIMPLE did on the IBM 4341, but SIMPLER consumed about 4 times the CPU times as SIMPLE did on FPS-264. Both algorithms computed the same results, but the SIMPLE algorithm requires less time for convergence. Consequently, the widely-used SIMPLE algorithm was selected for the computations in this research.

4.7 Summary

In this chapter, we presented the three-dimensional solution of the governing equations for the turbulent flow in three stirred tank systems. This solution was obtained from the nonisotropic model, and was validated by experimental data. Also, we compared the performance of three-dimensional nonisotropic and isotropic simulations which showed that the nonisotropic model is superior to the isotropic model. In addition, four two-dimensional simulations were compared with each other and with experimental data. We quantitatively showed that the two turbulence models proposed in this work described the flow more accurately than the models used by other investigators. Then a comparison of this research and previous studies was made. From this comparison, we found that a reliable method to provide the boundary conditions on the impeller periphery was necessary. The material balance had to be maintained for
the blade-swept region. Furthermore, data for turbulence kinetic energy and its dissipation rate were needed for quantitative comparisons. Also, the finite domain method was considered to be more flexible and promising than the stream function and vorticity transformations in the future research. Convergence and accuracy in the numerical approach was also discussed. Finally, we illustrated that the widely used SIMPLE algorithm was more efficient for this research than the SIMPLER algorithm.
4.8 References

5.1 Conclusions

In this research we reached the following conclusions:

1. The three-dimensional solution of the governing equations with the nonisotropic turbulence model was validated with experimentally measured velocity profiles and it was demonstrated that the flow was not symmetrical because of the baffles which reduce the rotational flow and increase the vertical flow. Also, there was circulation behind the baffles.

2. The three-dimensional solution for the turbulence kinetic energy and its dissipation rate from the nonisotropic simulation were qualitatively confirmed by the experimental data of the turbulence intensity and energy dissipation rate. These results showed that the impeller stream contained and consumed most turbulence kinetic energy in agitated vessels.

3. The flowfield from the three-dimensional isotropic model was significantly different than the flowfield from the three-dimensional nonisotropic model, and the isotropic model did not describe the flow in agitated vessels.

4. The computed velocity and turbulence fields showed that there was symmetry in the region of the jet zone close to the impeller. The flow
from the impeller dominated this region and overrode effects from the baffles, tank wall, and the flow in bulk regions.

5. There was an increase in computer time from the two-dimensional simulations to the three-dimensional simulations of the turbulent flow in agitated vessels. However, the two-dimensional solutions may be used to analyse processes which are important in the flow in the impeller jet zone for a savings in computational effort.

6. The two-dimensional simulation results should be used as the initial estimates for the three-dimensional calculations to reduce the CPU time required for convergence to a solution.

7. In two-dimensional simulation, ability of the isotropic model to describe the flow was improved significantly by artificially adding drag terms in the angular momentum equation. This reduced the tangential velocity to account for the baffling effects. The other two velocity components were indirectly affected by this reduced tangential velocity.

8. The finite domain method was successfully employed in this research. This method was easily extended from two dimensions to three dimensions. A major achievement of this research has been the development of a general purpose three-dimensional computer code using this method to solve simultaneous partial differential equations.

9. The SIMPLE and SIMPLER algorithms were applied to two-dimensional flow systems in agitated vessels. The results showed that the SIMPLE algorithm was more efficient to obtain converged solutions for the turbulent flow in agitated vessels.
5.2 Recommendations

The following recommendations are made based upon this research:

1. Additional experimental measurements are needed for velocities, turbulence kinetic energy and its dissipation rate throughout the tank and in the impeller region. Data for the turbulence kinetic energy and dissipation rate are especially needed, since there has been no detailed experimental study for the turbulence kinetic energy and its dissipation rate.

2. More experimental studies on the flow around the impeller are needed, especially at the impeller tip and on the top and bottom sides of the blades. These results may be used to provide complete boundary conditions, and thus zero-gradient assumptions for the blade-swept region can be eliminated.

3. The solution should be extended to other tank and impeller sizes to determine the scale-up capability. Also, the computed velocity profiles and the eddy viscosity distribution can be applied in many processes. For example, in fermentation processes the shear rate and shear stress are the major process concern; and in some suspension processes there is a special interest in the axial velocity distribution.

4. This research can be expanded to study theoretically applications in agitated vessels by including the transport equations associated with those applications. For example, in previous research concerning dispersions, the convective terms in the species continuity equations were purposely neglected by assuming that the velocity vector and concentration gradient vector were orthogonal in the interface, and thus the intractable flowfield calculations could be bypassed. Now we
have established a turbulent fluid dynamic simulation for the flowfield in agitated vessels, and the above-mentioned assumption can then be eliminated. For this type of research, the two-dimensional simulation with our nonisotropic turbulence model should provide a good starting point. This is because it takes much less CPU time to obtain results that are approximate to the three-dimensional simulation.

5. The nonisotropic turbulence model is promising because of its flexibility in having different viscosity components at the same point. It is worthwhile to examine the consequences of having different expressions for the viscosity ratios. In this research, we only allowed one of five viscosity ratios to be various locally and held the other four constant.

6. It would be very interesting to apply the nonisotropic model to study the two-dimensional flow patterns in jet-stirred reactors.
Nomenclature

English

A  A tangential jet parameter (Equation II-14)
A  Area
A  Coefficient
A  Expression of convection-diffusion term
a  A tangential jet parameter (Equation II-13)
a  Ring source radius
a  Empirical constant
a  Coefficient used in TDMA (Equation III-125)
b  Related to the control face on bottom side
b  Empirical constant
b  Coefficient used in TDMA (Equation III-125)
C  Coefficient in discretization equations
C_1  Turbulence model coefficient (Equation III-35)
C_2  Turbulence model coefficient (Equation III-36)
C_c  Turbulence model coefficient (Equation III-40)
C_\mu  Turbulence model coefficient (Equation III-34)
C_{Dr}  Drag coefficient
C_{Drb}  Drag coefficient for bulk region
C_{Drj}  Drag coefficient for jet zone
c  Coefficient used in TDMA (Equation III-125)
D  Viscous diffusion term
D_I  Impeller diameter
D_r  Drag term
$D_T$ Tank diameter

d Coefficient used in TDMA (Equation III-125)
e Related to the control face on east side
f fraction
G Production term in the turbulence energy equation
$G_P$ Production term for $k_p$ by Placek, et al. (12, Chapter II)
$G_r$ Radial flux of radial momentum
$G_\theta$ Radial flux of angular momentum
g Gravitational constant
$g_c$ Conversional factor
$H_b$ Width of impeller blade
$H_1$ Impeller height from tank bottom
$H_2$ Liquid height
$I$ Related to the axial coordinate
$J$ Related to the radial coordinate
$K_1$ Empirical constant (Equation I-8)
$K_2$ Empirical constant (Equation I-9)
$K_3$ Empirical constant (Equation I-10)
k Turbulence kinetic energy
$k$ Proportional constant of stagnant inner core to impeller radius
$k'$ Nondimensionalized turbulence kinetic energy
$k_p$ Turbulence kinetic energy for large scale vortices
$k_T$ Turbulence kinetic energy for transfer eddies
$M$ Recurrence relation in TDMA
$N$ Recurrence relation in TDMA
N Impeller rotation speed
$N_{Fr}$ Froude number
$N_{Re}$ Reynolds number
\( N_p \)  Power number
\( N_p \)  Peclet number
\( n \)  Related to the control face on north side
\( P \)  Power (Equation I-6)
\( \bar{P} \)  Time-averaged pressure
\( \tilde{P} \)  Pressure
\( P \)  Related to the main grid point
\( P' \)  Pressure correction
\( p \)  Fluctuating component of pressure
\( R \)  Impeller radius
\( R_k \)  Turbulent Reynolds number (Equation III-37)
\( R_t \)  Turbulent Reynolds number (Equation III-33)
\( R_{it} \)  Turbulent Richardson number (Equation III-39)
\( r \)  Radial coordinate
\( \tilde{r} \)  Nondimensionalized radial coordinate
\( \varphi \)  Swirl number
\( S_\phi \)  Source term
\( s \)  Related to the control face on south side
\( t \)  Time
\( \tilde{t} \)  Related to the control face on top side
\( U \)  Time-averaged axial velocity
\( U' \)  Nondimensionalized time-averaged axial velocity
\( u \)  Fluctuating component of axial velocity
\( V \)  Time-averaged radial velocity
\( V' \)  Nondimensionalized time-averaged radial velocity
\( \tilde{V} \)  Velocity vector
\( V_r \)  Radial velocity
\( V_{tip} \)  Tip velocity
\( V_z \) Axial velocity
\( V_\theta \) Tangential velocity
\( v \) Fluctuating component of radial velocity
\( W \) Time-averaged tangential velocity
\( W' \) Nondimensionalized time-averaged tangential velocity
\( W_d \) Baffle width
\( w \) Fluctuating component of tangential velocity
\( w \) Related to the control face on west side
\( x \) Empirical constant (Equation I-11)
\( x_w \) Axial distance measured from tank bottom or liquid surface
\( y \) Empirical constant (Equation I-11)
\( y \) Radial distance measured from the centerline of the tank
\( y_w \) Radial distance measured from the tank wall
\( z \) Axial coordinate
\( z' \) Nondimensionalized axial coordinate

**Greek Letters**
\( \alpha \) Proportional constant (Equations III-136,137)
\( \beta \) Relaxation factor
\( \Delta \) Difference between control faces
\( \delta \) Difference between grid points
\( \varepsilon \) Turbulence energy dissipation rate
\( \varepsilon' \) Nondimensionalized turbulence energy dissipation rate
\( \eta \) A tangential jet parameter (Equation II-10)
\( \Gamma \) Exchange coefficient (Equations III-59,99)
\( \Lambda \) Macroscale of turbulence
\( \mu \) Fluid viscosity
\( \mu_t \) Turbulent viscosity
\( \nu_t \) Kinematic turbulent viscosity
\( \phi \) Variable
\( \rho \) Fluid density
\( \Sigma \) Summation
\( \sigma \) Tangential jet parameter (Equation II-12)
\( \sigma \) Prandtl-Schmidt number
\( \tau \) Turbulent stress tensor
\( \theta \) Tangential coordinate in radians
\( \theta' \) Tangential coordinate in degrees
\( \theta_y \) Angle at which velocity vector emerges from impeller tip

Superscript

* Previous iterative values

Subscripts

B Related to the grid point on bottom side
B Related to the boundary point
b Related to the control face on bottom side
E Related to the grid point on east side
e Related to the control face on east side
eff Effective value
I First interior grid point
I,J,K Related to coordinates in finite difference form
i Index of integers
i,j Related to coordinates in tensor form
i,j,k Related to coordinates in finite difference form
KPT Number of grid point in the \( \theta \)-direction
k Turbulence kinetic energy
max  Maximum value
N   Number of grid points
n   Related to the grid point on north side
nb  Related to the neighbouring points or faces
non Nonisotropic value
P   Related to the main grid point
R   Related to the impeller tip
r,θ,z Related to cylindrical coordinates
rz, etc. rz-component of second order tensor, etc.
S   Related to the grid point on south side
s   Related to the control face on south side
T   Related to the grid point on top side
t   Related to the control face on top side
W   Related to the grid point on west side
w   Related to the control face on west side
ε   Turbulence energy dissipation rate
φ   Variable
Appendix A:

Material Balance over the Blade-Swept Region

The calculation procedure used to obtain the proportional constant \( a \) in equations (III-136) and (III-137) is given here by performing a material balance over the blade-swept region shown in Figure III-1. The inflow to this region is given in terms of the discretized axial velocities \( U(I_T, J) \) and \( U(I_B, J) \) which are on the horizontal faces of the impeller.

\[
\text{Inflow} = \sum_{J=2}^{J_R} \left[ \rho(I_T, J)|U(I_T, J)|A(I_T, J) + \rho(I_B, J)|U(I_B, J)|A(I_B, J) \right]
\]

The outflow from this region is given in terms of the discretized radial velocity \( V(I, J_R) \) on the plane circling the impeller tip.

\[
\text{Outflow} = \sum_{I=I_B}^{I_T} \rho(I, J_R)V(I, J_R)A(I, J_R)
\]

In these two equations \( A \) is the area of the control surface, \( \rho \) is the liquid density, \( V(I, J_R) \) is the radial velocity on the impeller tip which is obtained from the tangential jet, and \( U(I_T, J) \) and \( U(I_B, J) \) are the axial velocity components on the top and bottom faces of the impeller blades which are unknown.

From a material balance for the steady flow of an incompressible fluid, the flow into the top and bottom of the impeller is equal to the flow out from the impeller tip, and the following equation is obtained:
\[ \sum_{I=I^T}^{I=I_B} V(I,J_R)A(I,J_R) = \sum_{J=2}^{J_R} \left[ |U(I,T,J)|A(I,T,J) + |U(I,B,J)|A(I,B,J) \right] \] (A-1)

The above equation involves two sets of unknowns, \( U(I,T,J) \) and \( U(I_B,J) \) on the right hand side of equation (A-1).

A procedure to follow would be to have this set of two unknown axial velocities be equal to the axial velocities on the planes one step above and below the impeller. This is called the zero-gradient assumption for the axial velocity. However, this would neglect the radial flow between these planes and the planes at the top and bottom of the impeller, and a material balance on the impeller would not be satisfied.

A convenient procedure to satisfy the material balance was developed to obtain the boundary conditions for the axial velocity components on the top and bottom side of the impeller by using a proportional constant as below.

\[ U(I_T,J) = \alpha U(I_T+1,J) \] \hspace{1cm} (III-136)

and

\[ U(I_B,J) = \alpha U(I_B-1,J) \] \hspace{1cm} (III-137)

where \( \alpha \) is a proportional constant. \( U(I_T+1,J) \) and \( U(I_B-1,J) \) are adjacent axial velocities to the \( U(I_T,J) \) and \( U(I_B,J) \), and they are on the plane above and below the impeller. \( U(I_T+1,J) \) and \( U(I_B-1,J) \) are given by the latest iterated values. If we know the proportional constant \( \alpha \), the axial velocities on the top and bottom faces can be obtained from equations (III-136) and (III-137) as the boundary condition there.

To obtain \( \alpha \), we have to substitute equations (III-136) and (III-137) into equation (A-1). The rearrangement will give the following equation for \( \alpha \):
\[ \alpha = \frac{\sum_{I=I_B}^{I_T} V(I,J_R)A(I,J_R)}{\sum_{J=2}^{J_R} [|U(I_T+1,J)|A(I_T,J)+|U(I_B-1,J)|A(I_B,J)]} \]  

In Table A-1, the calculated values of \( \alpha \) from four different two-dimensional simulations for three stirred tank systems are given and they range from 0.845 to 0.935. This means that the material balance for the blade-swept region would not be satisfied with the zero-gradient assumption \((\alpha=1)\) for the axial velocities on the top and bottom faces of the impeller. The average values of \( \alpha \) for each tank system are 0.850, 0.931, and 0.931, respectively, and the \( \alpha \)'s for Tank System 2 and Tank System 3 are almost the same for each turbulence model which is probably due to the same impeller diameter being used in these two tank systems. It is not necessary that they be equal, because \( \alpha \) also varies with impeller speeds. These average values of \( \alpha \) in Table A-1 were used in the three-dimensional simulations.
Table A-1. The Computed Values of Proportional Constant $\alpha$ from the Two-Dimensional Simulations.

<table>
<thead>
<tr>
<th>Tank System $^\alpha$</th>
<th>Model $^\square$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>Model Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>0.845</td>
<td>0.928</td>
<td>0.928</td>
<td>Isotropic, Swirling, Baffling</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.847</td>
<td>0.930</td>
<td>0.929</td>
<td>Nonisotropic, Swirling, Baffling</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.855</td>
<td>0.929</td>
<td>0.929</td>
<td>Isotropic, Baffling</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>0.854</td>
<td>0.935</td>
<td>0.936</td>
<td>Isotropic</td>
</tr>
<tr>
<td>Average</td>
<td></td>
<td>0.850</td>
<td>0.931</td>
<td>0.931</td>
<td></td>
</tr>
</tbody>
</table>

$^\square$: Four different k-\(\varepsilon\) turbulence models were used in the two-dimensional simulations. Summary of these four turbulence models was given in Table IV-3.

$^\alpha$: Three tank systems were given in Table IV-1. Tank System 1 is a 11.5-inch tank with a 3-inch impeller at 250 rpm, Tank Systems 2 and 3 are an 11.5-inch tank with a 4-inch impeller at 150 and 200 rpm, respectively.
Appendix B:

Figures for Tank Systems 2 and 3

In this appendix figures are included for the turbulence kinetic energy and its dissipation rate for Tank System 2 and Tank System 3. The figures showing the effects of drag terms on the three velocity components for Tank Systems 2 and 3 are also included. These figures provide comparable information to those given in Chapter IV for Tank System 1.
Figure B-1. Turbulence kinetic energy of the impeller stream on the r-θ plane in Tank System 2.
Figure B-2. Turbulence kinetic energy of the impeller stream on the r-θ plane in Tank System 3.
Figure B-3. Contours of turbulence kinetic energy on the 45° plane in Tank System 2.
Figure B-4. Block diagrams of turbulence kinetic energy on the 45° plane in Tank System 2.
Figure B-5. Contours of turbulence kinetic energy on the 45° plane in Tank System 3.
Figure B-6. Block diagrams of turbulence kinetic energy on the 45° plane in Tank System 3.
Figure B-7. Energy dissipation rate of the impeller stream on the r-θ plane in Tank System 2.
Figure B-8. Energy dissipation rate of the impeller stream on the r-θ plane in Tank System 3.
Figure B-9. Contours of energy dissipation rates on the 45° plane in Tank System 2.
(a) Front view

(b) Back view

Figure B-10. Block diagrams of dissipation rates on the 45° plane in Tank System 2.
Figure B-11. Contours of energy dissipation rates on the 45° plane in Tank System 3.
Figure B-12. Block diagrams of dissipation rates on the 45° plane in Tank System 3.
Figure B-13. The drag effects on velocity in the bulk region of Tank System 2. The number on the left in parenthesis is $C_{Drj}$, and the one on the right is $C_{Drb}$. 
Figure B-14. The drag effects on velocity in the jet zone of Tank System 2. The number on the left in parenthesis is $C_{D_{rj}}$, and the one on the right is $C_{D_{rb}}$. 
Figure B-15. The drag effects on velocity in the bulk region of Tank System 3. The number on the left in parenthesis is $C_{Drj}$, and the one on the right is $C_{Drb}$. 
Figure B-16. The drag effects on velocity in the jet zone of Tank System 3. The number on the left in parenthesis is $C_{Drj}$, and the one on the right is $C_{Drb}$. 
Appendix C:

Program Listing

This appendix gives the three-dimensional computer program used in this research. The notation of variables in the program are also included.
Listing of FORTRAN variables

COMMON/ALGTHM/
    SIMPLE  Indicating SIMPLE algorithm.

COMMON/BAFFLE/
    JBAFFL  Radial position of baffles.

COMMON/BCPLL/
    UIBC    Axial velocity at impeller tip.
    VIBC    Radial velocity at impeller tip.
    WIBC    Tangential velocity at impeller tip.

COMMON/BIGNUM/
    BIG     A big number 1.0D30.

COMMON/CALN/
    CIM     Coefficients in the discretization equations.
    CIP     Coefficients in the discretization equations.
    CJM     Coefficients in the discretization equations.
    CJP     Coefficients in the discretization equations.
    CKM     Coefficients in the discretization equations.
    CKP     Coefficients in the discretization equations.
    CON     Source terms in the discretization equations.
    CP      Coefficients in the discretization equations.

COMMON/DEN/
    RHOCON  Constant density.

COMMON/FIRST/
    IST     First internal point in i-direction.
    JST     First internal point in j-direction.
    KST     First internal point in k-direction.

COMMON/FIRST1/
IST1  IST-1
JST1  JST-1
KST1  KST-1

COMMON/GAMLAM/
ZMUL  Laminar viscosity.

COMMON/GAM2/
NOTURB  Indicating non-turbulent flow systems.
ONCE  Indicating one time only.

COMMON/GRDTYP/
UNIFOM  Indicating uniform grid.

COMMON/ITER1/
DT  The time step.
ITER  A counter for iterations.
LAST  A maximum number of iterations.
TIME  Time in unsteady cases.

COMMON/LAXDT/
DTLAX  Relaxation time.

COMMON/LAXSOR/
RELSOR  Relaxation factors for source terms.

COMMON/LAXVAR/
RELAX  Relaxation factors for equations.

COMMON/LAX2/
ITRLAX  A counter for iterations to change relaxation factors.
NCHNGE  A total number for changing relaxation factors.

COMMON/LAX3/
DBETA  Changes in relaxation factors.

COMMON/NODES/
ARX  The area of main control volume face normal to i-direction.
ARXJ Part of ARX.
ARXJP The other part of ARX.
R Radial position of grid point.
RMN Radial position of control faces.
VOLM Volume of main finite domain.
VOLU Volume of finite domain for axial velocity.
VOLV Volume of finite domain for radial velocity.
VOLW Volume of finite domain for tangential velocity.
X Axial position of grid points.
XDF Spacing between control faces in i-direction.
XDFI Part of XDF.
XDFIP The other part of XDF.
XDG Spacing between grid points in i-direction.
XDSG Staggered counterpart of XDG.
XU Axial position of control faces.
Y The values of Y at grid points.
YDF Spacing between control faces in j-direction.
YDFR Product of R and YDF; Area for main finite domains.
YDG Spacing of grid points in j-direction.
YDSG Staggered counterpart of XDSG.
YD SGR Product of R and YDSG; Area for staggered finite domains.
YV Radial position of control faces.
YW Radial distance from the wall.
Z Tangential position of grid points.
ZDF Spacing between control faces in k-direction.
ZDFK Part of ZDF.
ZDFKP The other part of ZDF.
ZDG Spacing between grid points in k-direction.
ZDSG  Staggered counterpart of ZDG.
ZW    Tangential position of control faces.

COMMON/NPTS/
  IPT   Total grid points in i-direction.
  IPT1  IPT-1
  IPT2  IPT-2
  JPT   Total grid points in j-direction.
  JPT1  JPT-1
  JPT2  JPT-2
  KPT   Total grid points in k-direction.
  KPT1  KPT-1
  KPT2  KPT-2

COMMON/NSWEEP/
  NISP   The number to sweep in i-direction.
  NJSP   The number to sweep in j-direction.
  NKSP   The number to sweep in k-direction.

COMMON/NTIME1/
  NTIMES The number of repetitions of the sweeps in all directions.

COMMON/NUMBER/
  MAXVAR A maximum number to store variables.
  NGAM   The number representing exchange coefficients.
  NK     The number representing turbulence energy.
  NK2    The number representing dissipation rate.
  NP     The number representing pressure.
  NPC    The number representing pressure correction.
  NRHO   The number representing density.
  NRW    The number representing RW.
  NU     The number representing U.
NV   The number representing V.
NVAR The number representing some variable.
NW   The number representing W.
NZMUT The number representing turbulent viscosity.

COMMON/OVERFL/
OVFLW A number to prevent overflow.

COMMON/PAI/
PI   3.1417.

COMMON/PELLER/
DIMPEL Impeller diameter.
RPM   Impeller speed.

COMMON/PEXTPO/
PBCEXT Indicating the extrapolation of P to boundaries.

COMMON/POUT/
IPREF Reference point for pressure in i-direction.
JPREF Reference point for pressure in j-direction.
KPREF Reference point for pressure in k-direction.

COMMON/PRESS/
DRW   Coefficient in velocity correction for RW.
DU    Coefficient in velocity correction for U.
DV    Coefficient in velocity correction for V.

COMMON/PROP/
GAMIE D Viscosity at the i-direction edge of the finite domain.
GAMI WT Viscosity at the position where U resides.
GAMJE D Viscosity at the j-direction edge of the finite domain.
GAMJW T Viscosity at the position where V resides.
GAMK E D Viscosity at the k-direction edge of the finite domain.
GAMKWT Viscosity at the position where W resides.
RHOIED  Density at the i-direction edge of the finite domain.
RHOIWT  Density at the position where U resides.
RHOJED  Density at the j-direction edge of the finite domain.
RHOJWT  Density at the position where V resides.
RHOKED  Density at the k-direction edge of the finite domain.
RHOKWT  Density at the position where W resides.

COMMON/PRT/
PRNT    Print results of some variables.

COMMON/PRTRES/
PRESDU  Print residuals.

COMMON/PWRL/
CD      Combined effects of convection and diffusion.
DIFF    Diffusive flux.
FLOW    Convective flow.

COMMON/QUIT/
CONVGN  Convergent.

COMMON/RHOV/
RHOVAR  Various density.

COMMON/SHAPE/
XL      Calculation domain size in i-direction.
YL      Calculation domain size in j-direction.
ZL      Calculation domain size in k-direction.

COMMON/SDLN/
SOLVE   Solve for some variables.

COMMON/SOLVST/
NSOLST  The first variable to be solved.

COMMON/SORTUR/
CMU     $C_\mu$ in the turbulence model.
RT  Turbulence Reynolds number.
COMMON/SOR1/
GC  Conversion factor for gravitational constant.
GZ  Gravitational constant.
PATM Atmospheric pressure.
COMMON/SUMAX/
CONTMX Maximum residue of continuity equation for finite domains.
CONTOT Total residue of cont. eqn. for entire calculation domain.
RESMAX Maximum residue of transport equations for finite domains.
COMMON/TITLE1/
TITLE Title associated with some particular variable.
COMMON/VARS/
GAM  Exchange coefficient
P  Pressure
PC  Pressure correction
RHO  Density
RW  Angular momentum
U  Axial velocity
V  Radial velocity
VAR  Some particular variable
W  Tangential velocity
ZK  Turbulence kinetic energy
ZK2  Dissipation rate of turbulence energy
ZMUT  Turbulent viscosity
COMMON/VELAVG/
UJAVG Average of U at the k-direction edge of the finite domain.
UKAVG Average of U at the j-direction edge of the finite domain.
VIAVG Average of V at the k-direction edge of the finite domain.
VKAVG  Average of V at the i-direction edge of the finite domain.
WIAVG  Average of W at the j-direction edge of the finite domain.
WJAVG  Average of W at the i-direction edge of the finite domain.

COMMON/VELHAT/
UHEAD  Hat velocity U
VHEAD  Hat velocity V
WHEAD  Hat velocity W

COMMON/WTING/
FX  Interpolation factors for density in i-direction.
FXM  Interpolation factors for density in i-direction.
FY  Interpolation factors for density in j-direction.
FYM  Interpolation factors for density in j-direction.
FV  Interpolation factors for the mass flow in j-direction.
FVP  Interpolation factors for the mass flow in j-direction.
FZ  Interpolation factors for density in k-direction.
FZM  Interpolation factors for density in k-direction.
IMPLICIT REAL*8 (A-H,O-Z)

C --- THIS PROGRAM WAS DESIGNED TO SOLVE THE THREE-DIMENSIONAL
C --- PARTIAL DIFFERENTIAL TRANSPORT EQUATIONS IN CYLINDRICAL
C --- COORDINATE. IT WAS SUCCESSFULLY EXECUTED ON BOTH IBM 3084
C --- AND FPS-264 SCIENTIFIC COMPUTER.
C --- SHENG-YANG JU AT LOUISIANA STATE UNIVERSITY
C --- FALL 1982 -- SUMMER 1987

LOGICAL CONVGN
COMMON/QUIT/ CONVGN
CALL DOMAIN
CALL INITIA
100 CALL BCS
CALL RESULT
IF(CONVGN) STOP
CALL EQNS
GO TO 100
END

SUBROUTINE RESULT

A SUBROUTINE TO ARRANGE THE RESULTS FOR PRINTING

IMPLICIT REAL*8 (A-H,O-Z)
LOGICAL CONVGN,PRNT,PBCEXT
DIMENSION VWU(30,26,25)
COMMON/PRT(PRNT(14)
CHARACTER*15 TITLE
COMMON/TITLE/TITLE(14)
COMMON/SHAPE/ XL,YL,ZL
COMMON/PELLER/ DIPMEL,RPM
COMMON/PAI/ PI
COMMON/QUIT/ CONVGN
COMMON/VARS/ VAR(30,26,25,14)
COMMON/PROP/RH0IWT(30,26,25),RHOJW7(30,26,25),RHOKWT(30,26,25),
& GAM0WT(30,26,25),GAMJW7(30,26,25),GAMKWT(30,26,25),
& RHOIED(30,26,25),RHOJED(30,26,25),RHOKED(30,26,25),
& GAM0ED(30,26,25),GAMJED(30,26,25),GAMKED(30,26,25)
COMMON/NODES/
& X(30),XU(30),XDG(30),XDF(30),XDSC(30),
& Y(30),YV(30),YDG(30),YDF(30),YDSC(30),
& Z(30),ZW(30),ZDG(30),ZDF(30),ZDSC(30),
& YDFR(30),YDSGR(30),ARX(30),ARXJ(30),ARXJP(30),
& XDFI(30),XDFIP(30),ZDFK(30),ZDFKP(30),
& R(30),RMN(30),YW(30),
& VOLM(30,26,25), VOLV(30,26,25),
& VOLW(30,26,25), VOLU(30,26,25)
COMMON/WTING/
& FX(30),FXM(30),FY(30),FYM(30),FV(30),FVP(30),
& FZ(30),FZM(30)
COMMON/NUMBER/
& NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
& NV,NRW,NU,NPC,NP,NK,NK2
COMMON/ITER1/ ITER,LAST,TIME,DT
COMMON/NPTS/ IPT1,IPT2,JPT1,JPT2,KPT1,KPT2
COMMON/POUT/ IPREF,KPREF
COMMON/PEXTPO/ PBCEXT
DIMENSION U(30,26,25),V(30,26,25),PC(30,26,25),P(30,26,25),
& RW(30,26,25),W(30,26,25),ZK(30,26,25),ZK2(30,26,25),
& ZMUT(30,26,25),GAM(30,26,25),RH0(30,26,25)

EQUIVALENCE
& (VAR(1,1,1,1),V(1,1,1)),(VAR(1,1,1,2),RW(1,1,1)),
& (VAR(1,1,1,3),U(1,1,1)),
& (VAR(1,1,1,4),P(1,1,1)),(VAR(1,1,1,5),PC(1,1,1)),
& (VAR(1,1,1,6),ZK(1,1,1)),(VAR(1,1,1,7),ZK2(1,1,1))

EQUIVALENCE
& (VAR(1,1,1,11),W(1,1,1)),(VAR(1,1,1,12),ZMUT(1,1,1)),
& (VAR(1,1,1,13),GAM(1,1,1)),(VAR(1,1,1,14),RH0(1,1,1))

C
2 FORMAT(/15X,' Flow Field Modeling in a Stirred Tank '1,/
& 14X,41(1H*),//)
6 FORMAT(20X,' I',6X,'XU(I)',6X,'X(I)',/)
7 FORMAT(20X,I2,6X,' --- ','5X,F6.3)
8 FORMAT(20X,I2,2(5X,F6.3))
17 FORMAT(20X,I2,6X,' --- ','2(5X,F6.3))
18 FORMAT(20X,I2,3(5X,F6.3))
9 FORMAT(/,20X,' J',6X,'YV(J)',6X,'Y(J)',6X,'YW(J)',//)
19 FORMAT(/,20X,' K',6X,'ZW(K)',6X,'Z(K)',/)
10 FORMAT(/,1X,30(1H*),2X,AI5,2X,30(1H*))
11 FORMAT(/,1X,30(1H*),7X,'K = ',12,7X,30(1H*))
12 FORMAT(/,1X,' The following tabulated values are in SI Unit')
15 FORMAT(/,13X,' --- All pressure values are relative to P('',
& 12,' ',I2,' ',I2,' ') ---')
20 FORMAT(/,3X,' I='AI6.5I12)
30 FORMAT(1X,'J='2X,75X,'J=')
40 FORMAT(1X,I2,1X,1P,6E12.4,2X,I2)
31 FORMAT(1X,'J=')
41 FORMAT(1X,I2,1X,1P,6E12.4)

C
IF(ITER.EQ.0) THEN
WRITE(8,2)
C
--- Change units of X, XU, Y, YW, and YV from feet to INCHES ------
DO 310 I=1,IPT
   IF(I.GE.2) XU(I)=XU(I)*12.
310 X(I)=X(I)*12.
DO 330 J=1,JPT
   IF(J.GE.2) YV(J)=YV(J)*12.
   Y(J)=Y(J)*12.
330 YW(J)=YW(J)*12.
C
--- Change units of Z and ZW from radiants to DEGREES ------
DO 350 K=1,KPT
   IF(K.GE.2) ZW(K)=ZW(K)*180.0/PI
350 Z(K)=Z(K)*180.0/PI
C
WRITE(8,6)
DO 420 I=1,IPT
IF(I.EQ.1) THEN
   WRITE(8,7) I,X(I)
ELSE
   WRITE(8,8) I,XU(I),X(I)
END IF

WRITE(8,9)
DO 440 J=1,JPT
   IF(J.EQ.1) THEN
      WRITE(8,17) J,Y(J),YW(J)
   ELSE
      WRITE(8,18) J,YV(J),Y(J),YW(J)
   END IF
440 CONTINUE

WRITE(8,19)
DO 460 K=1,KPT
   ZDGTM = Z(K) - 1.0
   ZWDGTM = ZW(K) - 1.0
   IF(K.EQ.1) THEN
      WRITE(8,7) K,ZDGTMP
   ELSE
      WRITE(8,8) K,ZWDGTM,ZDGTM
   END IF
460 CONTINUE

C --- Change units of X, XU, Y, YW, and YV from inches to FEET ------
DO 311 I=1,IPT
   IF(I.GE.2) XU(I)=XU(I)/12.
   X(I)=X(I)/12.
311 DO 331 J=1,JPT
   IF(J.GE.2) YV(J)=YV(J)/12.
   Y(J)=Y(J)/12.
   YW(J)=YW(J)/12.
331 C --- Change units of Z and ZW from degrees to RADIANTS ------
DO 351 K=1,KPT
   IF(K.GE.2) ZW(K)=ZW(K)*PI/180.0
   Z(K)=Z(K)*PI/180.0
351 C ----------------------------------------
   CALL ITEREDE
C -----------------------------------
IF(CONVGN) THEN
C
   IF(PRNT(NRW)) THEN
      DO 50 K=1,KPT
         DO 50 J=1,JPT
         DO 50 I=1,IPT
            VAR(I,J,K,NRW)=W(I,J,K)
50      END IF
C
   IF(PRNT(NW)) THEN
      DO 60 K=1,KPT
         DO 60 J=1,JPT
C
DO 60 I=1,IPT
   VAR(I,J,K,NW)=GAM(I,J,K)/RHO(I,J,K)
END IF

C
IF(PRNT(NZMUT)) THEN
   DO 65 K=1,KPT
   DO 65 J=1,JPT
   DO 65 I=1,IPT
   VAR(I,J,K,NZMUT)=ZMUT(I,J,K)/RHO(I,J,K)
END IF

C
IF(PRNT(NV)) THEN
   DO 71 K=1,KPT
   DO 71 I=1,IPT
   VWU(I,1,K)=VAR(I,2,K,NV)
   VWU(I,JPT,K)=VAR(I,JPT,K,NV)
   DO 71 J=2,JPT1
   VWU(I,J,K)=0.5*(VAR(I,J+1,K,NV)+VAR(I,J,K,NV))
   CONTINUE
   DO 73 K=1,KPT
   DO 73 J=1,JPT
   DO 73 I=1,IPT
   VAR(I,J,K,NV)=VWU(I,J,K)
END IF

C
IF(PRNT(NRW)) THEN
   DO 74 J=1,JPT
   DO 74 I=1,IPT
   VWU(I,K,1)=VAR(I,J,2,NRW)
   VWU(I,J,KPT)=VAR(I,J,KPT,NRW)
   DO 74 K=2,KPT1
   VWU(I,J,K)=0.5*(VAR(I,J,K+1,NRW)+VAR(I,J,K,NRW))
   CONTINUE
   DO 78 K=1,KPT
   DO 78 J=1,JPT
   DO 78 I=1,IPT
   VAR(I,J,K,NRW)=VWU(I,J,K)
END IF

C
IF(PRNT(NU)) THEN
   DO 76 K=1,KPT
   DO 76 J=1,JPT
   VWU(1,J,K)=VAR(2,J,K,NU)
   VWU(IPT,J,K)=VAR(IPT,J,K,NU)
   DO 76 I=2,IPT1
   VWU(I,J,K)=0.5*(VAR(I+1,J,K,NU)+VAR(I,J,K,NU))
   CONTINUE
   DO 78 K=1,KPT
   DO 78 J=1,JPT
   DO 78 I=1,IPT
   VAR(I,J,K,NU)=VWU(I,J,K)
END IF
DO 70 NVAR=1,MAXVAR
   IF(PRNT(NVAR)) THEN
      IF(NVAR.EQ.NV .OR. NVAR.EQ.NRW .OR. NVAR.EQ.NU) CONVER=0.3048
IF(NVAR.EQ.NP) CONVER= 101330.0/2116.2
IF(NVAR.EQ.NK) CONVER= 0.3048*0.3048
IF(NVAR.EQ.NK2) CONVER= 0.3048*0.3048
IF(NVAR.EQ.NZMUT) CONVER= 0.3048*0.3048
IF(NVAR.EQ.NW) CONVER= 0.3048*0.3048
DO 80 K=1,KPT
DO 80 J=1,JPT
DO 80 I=1,IPT

80 VAR(I,J,K,NVAR)=VAR(I,J,K,NVAR)*CONVER
END IF

70 CONTINUE

IF(PRNT(NP)) THEN
IF(PBCEXT) THEN
DO 91 K=2,KPT
DO 91 J=2,JPT
P(I,J,K)=(P(I,J,K)*YDSG(3)-P(I,J,K)*YDSG(2))/YDSG(3)
91 P(I,J,K)=P(I,J,K)*YDSG(IPT1)-P(I,J,K)*YDSG(IPT)
& /YDSG(IPT1)
DO 92 K=2,KPT
DO 92 I=2,IPT
P(I,J,K)=(P(I,J,K)*YDSG(3)-P(I,J,K)*YDSG(2))/YDSG(3)
92 P(I,J,K)=P(I,J,K)*YDSG(IPT1)-P(I,J,K)*YDSG(IPT)
& /YDSG(IPT1)
DO 93 J=2,JPT
DO 93 I=2,IPT
P(I,J,K)=P(I,J,K)*ZDSG(3)-P(I,J,K)*ZDSG(2))/ZDSG(3)
93 P(I,J,K)=P(I,J,K)*ZDSG(KPT1)-P(I,J,K)*ZDSG(KPT)
& /ZDSG(KPT1)

END IF
DO 94 K=1,KPT
DO 94 J=1,JPT
DO 94 I=1,IPT

94 P(I,J,K)=P(I,J,K)-P(IPREF,JPREF,KPREF)
END IF

WRITE(8,12)
DO 202 K=1,KPT
DO 200 NVAR=1,MVVAR
IF(PRNT(NVAR)) THEN
WRITE(8,11) K
WRITE(8,10) TITLE(NVAR)
IF(NVAR.EQ.NP) WRITE(8,15) IPREF,JPREF,KPREF
IFST=1
JFST=1
IF(NVAR.EQ.NPC) IFST=2
IF(NVAR.EQ.NPC) JFST=2
IBEG=IFST-6
CONTINUE
IBEG=IBEG+6
IEND=(IBEG-1)+6
IEND=MIN0(IEND,IPT)
INUM=IEND-IBEG+1
WRITE(8,20) (I,I=IBEG,IEND)
IF(INUM.EQ.6) THEN
WRITE(8,30)
ELSE
WRITE(8,31)
END IF
DO 115 JJ=JFST,JPT
J=JFST+JPT-JJ
IF(INUM.EQ.6) THEN
WRITE(8,40) J,(VAR(I,J,K,NVAR),I=IBEG,IEND),J
ELSE
WRITE(8,41) J,(VAR(I,J,K,NVAR),I=IBEG,IEND)
END IF
115 CONTINUE
IF(IEND.LT.IPT) GO TO 110
ELSE
END IF
200 CONTINUE
202 CONTINUE
C
ELSE
END IF
RETURN
END
C
======================================================================
SUBROUTINE EQNS
C
C USE SIMPLE TO SOLVE EQUATIONS
C
IMPLICIT REAL*8 (A-H,O-Z)
LOGICAL SOLVE,CONVGN,PRESDU,SIMPLE
COMMON/QUIT/CONVGN
COMMON/ALGTHM/ SIMPLE
COMMON/SUMAX/CONTOT,CONTMX,RESMAX(14)
COMMON/PRTRES/PRESDU
COMMON/SOLN/SOLVE(14)
COMMON/LAXVAR/RELAX(14)
COMMON/VARS/ VAR(30,26,25,14)
COMMON/CALN/ CP(30,26,25),CON(30,26,25),
& CIP(30,26,25),CIM(30,26,25),
& CJP(30,26,25),CKM(30,26,25),
& CP(30,26,25)
COMMON/VELHAT/ UHEAD(30,26,25),VHEAD(30,26,25),WHEAD(30,26,25)
COMMON/NODES/
& X(30),XU(30),XDG(30),XDF(30),XDSG(30),
& Y(30),YV(30),YDG(30),YDF(30),YDSG(30),
& Z(30),ZW(30),ZDG(30),ZDF(30),ZDSG(30),
& YDFR(30),YDSGR(30),ARX(30),ARXJ(30),ARXJP(30),
& XDFI(30),XDFIP(30),ZDK(30),ZDFKP(30),
& R(30),RMN(30),YW(30),
& VOLM(30,26,25), VOLV(30,26,25),
& VOLW(30,26,25), VOLU(30,26,25)
COMMON/WT ING/
& FX(30),FXM(30),FY(30),FYM(30),FVP(30),
& FZ(30),FZM(30)
COMMON/PRESS/ DU(30,26,25),DV(30,26,25),DRW(30,26,25)
COMMON/NUMBER/
& NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
& W,NV,NRW,NU,NPC,NP,NK,NK2
COMMON/ITER1/ ITER,LAST,TIME,DT
COMMON/NPTS/ IPT,IPT1,IPT2,JPT,JPT1,JPT2,KPT,KPT1,KPT2
COMMON/FIRST/ IST,JST,KST
COMMON/POUT/ IPREF,JPREF,KPREF
DIMENSION U(30,26,25),V(30,26,25),PC(30,26,25),P(30,26,25),
& RW(30,26,25),W(30,26,25),ZK(30,26,25),ZK2(30,26,25),
& ZMUT(30,26,25),GAM(30,26,25),RHO(30,26,25)
EQUIVALENCE
& (VAR(1,1,1,1),V(1,1,1)),(VAR(1,1,1,2),RW(1,1,1)),
& (VAR(1,1,1,3),U(1,1,1)),
& (VAR(1,1,1,4),PC(1,1,1)),(VAR(1,1,1,5),ZK(1,1,1)),
& (VAR(1,1,1,6),ZK2(1,1,1))
EQUIVALENCE
& (VAR(1,1,1,11),ZK(1,1,1)),(VAR(1,1,1,12),ZMUT(1,1,1)),
& (VAR(1,1,1,13),GAM(1,1,1)),(VAR(1,1,1,14),RHO(1,1,1))
SOLVE(NP)=.FALSE.
Do 3001 NVAR=1,MAXVAR
    IST=2
    JST=2
    KST=2
    IF(SOLVE(NVAR)) THEN
        IF(NVAR.EQ.NV) THEN
            JST=3
            CALL COE芙
            Do 3151 K=KST,KPT1
            Do 3151 J=JST,JPT1
            Do 3151 I=IST,IPT1
               CON(I,J,K)=CON(I,J,K)
               +(P(I,J-1,K)-P(I,J,K))*CP(I,J,K)*DV(I,J,K)
            3151 CONTINUE
            CALL SWEEPS
        ELSE IF(NVAR.EQ.NRW) THEN
            KST=3
            CALL COEFW
            Do 3251 K=KST,KPT1
            Do 3251 J=JST,JPT1
            Do 3251 I=IST,IPT1
               CON(I,J,K)=CON(I,J,K)
            3251 CONTINUE
            CALL SWEEPS
            Do 3201 K=2,KPT
            Do 3201 I=1,IPT
W(I,1,K)=0.
DO 3201 J=2,JPT
   W(I,J,K)=VAR(I,J,K,NVAR)/R(J)
3201   CONTINUE
ELSE IF(NVAR.EQ.NU) THEN
   IST=3
   CALL COEFU
   DO 3351 K=KST,KPT1
      DO 3351 J=JST,JPT1
         DO 3351 I=IST,IPT1
            CON(I,J,K)=CON(I,J,K)
                       +(P(I-1,J,K)-P(I,J,K))*CP(I,J,K)*DU(I,J,K)
         CONTINUE
         CALL SWEEPS
      END DO
      ELSE IF(NVAR.EQ.NPC) THEN
         CALL COEFPC
         DO 3501 K=KST,KPT1
            DO 3501 J=JST,JPT1
               DO 3501 I=IST,IPT1
                  PC(I,J,K)=0.
               CONTINUE
               CALL SWEEPS
            END DO
            ELSE IF(MOD(ITER,5).EQ.O) THEN
               DO 3591 K=2,KPT1
                  DO 3591 J=2,JPT1
                     DO 3591 I=2,IPT1
                        IF (I.GE.3) U(I,J,K)=U(I,J,K)
                       &+DU(I,J,K)*(PC(I-1,J,K)-PC(I,J,K))
                        IF(J.GE.3) V(I,J,K)=V(I,J,K)
                       &+DV(I,J,K)*(PC(I,J-1,K)-PC(I,J,K))
                        IF(K.GE.3) THEN
                           RW(I,J,K)=RW(I,J,K)
                       &+DRW(I,J,K)*(PC(I,J,K-1)-PC(I,J,K))
                           W(I,J,K)=RW(I,J,K)/R(J)
                       END IF
                        P(I,J,K)=P(I,J,K)+PC(I,J,K)*RELAX(NP)
                     CONTINUE
                     ELSE
                        END IF
               CONTINUE
            ELSE
               CALL COEFOT
               CALL SWEEPS
               ELSE
               IF(NVAR.EQ.NPC .OR. PRESDU) CALL RESIDU
               ELSE
               END IF
3001   CONTINUE
TIME=TIME+DT
ITER=ITER+1
RETURN
SUBROUTINE COEFFS

CALCULATE COEFFICIENTS OF THE DISCRETIZATION EQUATIONS

IMPLICIT REAL*8 (A-H,O-Z)
LOGICAL SOLVE,SIMPLE
COMMON/ALGTHM/ SIMPLE
COMMON/SOLN/SOLVE(14)
COMMON/LAXSOR/RELSOR(14)
COMMON/LAXVAR/RELAX(14)
COMMON/PRWL/FLOW,DIFF,CD
COMMON/VARS/ VAR(30,26,25,14)
COMMON/CALN/ CP(30,26,25),CON(30,26,25),
& CIP(30,26,25),CIM(30,26,25),
& CJP(30,26,25),CJM(30,26,25),
& CKP(30,26,25),CKM(30,26,25)
COMMON/VELHAT/ UHEAD(30,26,25),VHEAD(30,26,25),WHEAD(30,26,25)
COMMON/VELAVG/ UJAVG(30,26,25),VIAVG(30,26,25),WIAVG(30,26,25),
& UKAVG(30,26,25),VKAVG(30,26,25),WKAVG(30,26,25)
COMMON/PROP/RHOIWT(30,26,25),RHOJWT(30,26,25),RHOKWT(30,26,25),
& GAMIWT(30,26,25),GAMJWT(30,26,25),GAMKWT(30,26,25),
& RHOIED(30,26,25),RHOJED(30,26,25),RHOKED(30,26,25),
& GAMIED(30,26,25),GAMJED(30,26,25),GAMKED(30,26,25)
COMMON/NODES/
& X(30),XU(30),XDG(30),XDF(30),XDSG(30),
& Y(30),YV(30),YDG(30),YDF(30),YDSG(30),
& Z(30),ZW(30),ZDG(30),ZDF(30),ZDSG(30),
& YDFR(30),YDSGR(30),ARX(30),ARXJ(30),ARXJP(30),
& XDFI(30),XDFIP(30),ZDFK(30),ZDFKP(30),
& R(30),RMN(30),YW(30),
& VOLM(30,26,25),VOLV(30,26,25),
& VOLW(30,26,25),VOLU(30,26,25)
COMMON/WTING/
& FX(30),FXM(30),FY(30),FYM(30),FV(30),FVP(30),
& FZ(30),FZM(30)
COMMON/PRESS/ DU(30,26,25),DV(30,26,25),DRW(30,26,25)
COMMON/NUMBER/
& NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
& NV,NRW,NU,NPC,NP,NK,NK2
COMMON/ITER1/ ITER,LAST,TIME,DT
COMMON/NPTS/ IPT, IPT2, JPT, JPT1, JPT2, KPT, KPT1, KPT2
COMMON/FIRST/ IST, JST, KST
COMMON/OVERFL/ OVFILW
DIMENSION U(30,26,25),V(30,26,25),PC(30,26,25),P(30,26,25),
& RW(30,26,25),W(30,26,25),ZK(30,26,25),ZK2(30,26,25),
& ZMUT(30,26,25),GAM(30,26,25),RHO(30,26,25)
EQUIVALENCE
& (VAR(1,1,1,1), V(1,1,1)), (VAR(1,1,1,2), RW(1,1,1)),
& (VAR(1,1,1,3), U(1,1,1)),
& (VAR(1,1,1,4), P(1,1,1)), (VAR(1,1,1,5), PC(1,1,1)),
& (VAR(1,1,1,6), ZK(1,1,1)), (VAR(1,1,1,7), ZK2(1,1,1))
EQUVALENCE
& (VAR(1,1,1,11),W(1,1,1)), (VAR(1,1,1,12),ZMUT(1,1,1)),
& (VAR(1,1,1,13),GAM(1,1,1)), (VAR(1,1,1,14),RHO(1,1,1))

DIMENSION UHEAD(30,26,25), VHEAD(30,26,25), WHEAD(30,26,25)

EQUVALENCE
& (VAR(1,1,1,8), UHEAD(1,1,1)), (VAR(1,1,1,9), VHEAD(1,1,1)),
& (VAR(1,1,1,10), WHEAD(1,1,1))

DIMENSION CONV(30,26,25), CONRW(30,26,25), CONU(30,26,25),
& CON(30,26,25), CONK(30,26,25), CONK2(30,26,25)

ENTRY COEFFV

--- Coefficients for the V equation ---

CALL GAMMA
CALL PROPWT

IF(ITER.EQ.0) CALL AVGWJ
IF(ITER.EQ.0) CALL AVGUJ
CALL SORV
CALL CFADD
IF(RELSOR(NVAR).EQ.1.) GO TO 121
RLSOR1 = 1. - RELSOR(NVAR)
DO 120 K = KST, KPT1
DO 120 J = JST, JPT1
DO 120 I = IST, IPT1
  IF(ITER.EQ.0) CONV(I,J,K) = CON(I,J,K)
  CON(I,J,K) = RELSOR(NVAR)*CON(I,J,K) + RLSOR1*CONV(I,J,K)
120  CONV(I,J,K) = CON(I,J,K)
121 CONTINUE

--- Change UNDERRELAXATION factor ---
CALL RELXTN
RLAX1 = 1. - RELAX(NVAR)

DO 102 K = KST, KPT1
DO 102 I = IST, IPT1
  FLOW = V(I,2,K)*RHO(I,1,K)
  DIFF = GAM(I,1,K)/YDF(2)
  CALL PWRLAW
  CJM(I,3,K) = CD + DMAX1(0.0D0, FLOW)
102  CJM(I,3,K) = CJM(I,3,K)*RMN(2)*XDF(I)*ZDF(K)

DO 103 J = JST, JPT1
DO 103 I = IST, IPT1
  FLOW = WJAVG(I,J,2)*RHOIED(I,J,2)
  DIFF = GAMIED(I,J,2)/(RMN(J)*ZDG(2))
  CALL PWRLAW
  CKM(I,J,2) = CD + DMAX1(0.0D0, FLOW)
103  CKM(I,J,2) = CKM(I,J,2)*YDSG(J)*XDF(I)

DO 105 K = KST, KPT1
DO 105 J=JST,JPT1
   FLOW=UJAVG(2,J,K)*RHOKED(2,J,K)
   DIFF=GAMKED(2,J,K)/XDG(2)
   CALL PWRLAW
   CIM(2,J,K)=CD+DMAX1(0.DO,FLOW)
   CIM(2,J,K)=CIM(2,J,K)*YDSGR(J)*ZDF(K)
DO 105 I=IST,JPT1
   FLOW=UJAVG(I+1,J,K)*RHOKED(I+1,J,K)
   DIFF=GAMKED(I+1,J,K)/XDG(I+1)
   CALL PWRLAW
   CIM(I+1,J,K)=CD+DMAX1(0.DO,FLOW)
   CIM(I+1,J,K)=CIM(I+1,J,K)-FLOW
   TEMP=YDSGR(J)*ZDF(K)
   CIM(I+1,J,K)=CIM(I+1,J,K)*TEMP
   CIP(I,J,K)=CIM(I,J,K)*TEMP
   IF(J.EQ.JPT1) THEN
     FLOW=R(JPT) *V(I,JPT,K)*RHO(I,JPT,K)
     DIFF=R(JPT) *GAM(I,JPT,K)/YDF(JPT1)
     ELSE
     FL=RMN(J) *V(I,J,K)*RHOJWT(I,J,K)
     FLP=RMN(J+1) *V(I,J+1,K)*RHOJWT(I,J+1,K)
     FLOW=FV(J)*FL+FVP(J)*FLP
     DIFF=R(J) *GAM(I,J,K)/YDF(J)
     END IF
   CALL PWRLAW
   CJM(I,J+1,K)=CD+DMAX1(0.DO,FLOW)
   CJM(I,J+1,K)=CJM(I,J+1,K)-FLOW
   TEMP=XDF(I)*ZDF(K)
   CJM(I,J+1,K)=CJM(I,J+1,K)*TEMP
   CJP(I,J,K)=CJP(I,J,K)*TEMP
   FLOW=WJAVG(I,J,K+1)*RHOIED(I,J,K+1)
   DIFF=GAMIED(I,J,K+1)/(RMN(J)*ZDG(K+1))
   CALL PWRLAW
   CKM(I,J,K+1)=CD+DMAX1(0.DO,FLOW)
   CKP(I,J,K)=CKM(I,J,K+1)-FLOW
   TEMP=YDSGR(J)*XDF(I)
   CKM(I,J,K+1)=CKM(I,J,K+1)*TEMP
   CKP(I,J,K)=CKP(I,J,K)*TEMP
   APT=(RHO(I,J,K)*ARXJ(J)
    & +RHO(I,J-1,K)*ARXJP(J-1))/(YDSGR(J)*DT)
   CP(I,J,K)=CP(I,J,K)-APT
   CON(I,J,K)=CON(I,J,K)+APT*V(I,J,K)
   CP(I,J,K)=(-CP(I,J,K)*VOLV(I,J,K)
    & +CIP(I,J,K)+CIM(I,J,K)+CJP(I,J,K)
    & +CJM(I,J,K)+CKP(I,J,K)+CKM(I,J,K))/RELAX(NVAR)
   CON(I,J,K)=CON(I,J,K)*VOLV(I,J,K)
   DV(I,J,K)=VOLV(I,J,K)/(YDG(J)*CP(I,J,K))
105 CONTINUE
RETURN
C
ENTRY COEFRW

--- Coefficients for the RW equation -----

CALL AVGVK
CALL AVGUK

CALL SORRW
CALL CFFADD

IF(RELSOR(NVAR).EQ.1.) GO TO 221
RLSOR1 = 1.-RELSOR(NVAR)
DO 220 K=KST,KPT1
DO 220 J=JST,JPT1
DO 220 I=IST,IPT1

IF(ITER.EQ.0) CONRW(I,J,K)=CON(I,J,K)
CON(I,J,K)=RELSOR(NVAR)*CON(I,J,K)
& +RLSOR1*CONRW(I,J,K)
220 CONRW(I,J,K)=CON(I,J,K)
221 CONTINUE

--- Change UNDERRELAXATION factor ----

CALL RELXTN
RLAX1 = 1.-RELAX(NVAR)

DO 202 K=KST,KPT1
DO 202 I=IST,IPT1

FLOW=VKAVG(I,2,K)*RHOIED(I,2,K)
DIFF=GAMIED(I,2,K)/YDG(2)

CALL PWRLAW
CJM(I,2,K)=CD+DMAXI(0.D0,FLOW)
202 CJM(I,2,K)=CJM(I,2,K)*RMN(2)*XDF(I)*ZDSG(K)

DO 203 J=JST,JPT1
DO 203 I=IST,IPT1

FLOW=W(I,J,2)*RHO(I,J,1)
DIFF=GAM(I,J,1)/(R(J)*ZDF(2))

CALL PWRLAW
CKM(I,J,3)=CD+DMAXI(0.D0,FLOW)
203 CKM(I,J,3)=CKM(I,J,3)*YDF(J)*XDF(I)

DO 205 K=KST,KPT1
DO 205 J=JST,JPT1

FLOW=UKAVG(2,J,K)*RHOJED(2,J,K)
DIFF=GAMJED(2,J,K)/XDG(2)

CALL PWRLAW
CIM(2,J,K)=CD+DMAXI(0.D0,FLOW)

CIM(2,J,K)=CIM(2,J,K)*ARX(J)*ZDSG(K)
DO 205 I=IST,IPT1

FLOW=UKAVG(I+1,J,K)*RHOJED(I+1,J,K)
DIFF=GAMJED(I+1,J,K)/XDG(I+1)

CALL PWRLAW
CIM(I+1,J,K)=CD+DMAXI(0.D0,FLOW)

CIP(I,J,K)=CIM(I+1,J,K)-FLOW
TEMP= ARX(J)*ZDSG(K)
CIM(I+1,J,K)=CIM(I+1,J,K)* TEMP
CJP(I,J,K)=CJP(I,J,K)* TEMP

FLOW=VKAVG(I,J+1,K)*RHOIED(I,J+1,K)
DIFF=GAMIED(I,J+1,K)/YDG(J+1)
CALL PWRLAW
CJM(I,J+1,K)=CD+DMAX1(0.DO,FLOW)
CJP(I,J,K)=CJM(I,J+1,K)-FLOW
TEMP=RMN(J+1)*XDF(I)*ZDSG(K)
CJM(I,J+1,K)=CJM(I,J+1,K)* TEMP
CJP(I,J,K)=CJP(I,J,K)* TEMP

IF(K.EQ.KPT) THEN
FLOW=W(I,J,KPT)*RHO(I,J,KPT)
DIFF=GAM(I,J,KPT)/(R(J)*ZDF(K))
ELSE
FL=W(I,J,K)*RHOKWT(I,J,K)
FLP=W(I,J,K+1)*RHOKWT(I,J,K+1)
FLOW=0.5*(FL+FLP)
DIFF=GAM(I,J,K)/(R(J)*ZDF(K))
END IF
CALL PWRLAW
CKM(I,J,K+1)=CD+DMAX1(0.DO,FLOW)
CKP(I,J,K)=CKM(I,J,K+1)-FLOW
TEMP=YDF(J)*XDF(I)
CKM(I,J,K+1)=CKM(I,J,K+1)* TEMP
CKP(I,J,K)=CKP(I,J,K)* TEMP

APT=RHOKWT(I,J,K)/DT
CP(I,J,K)=CP(I,J,K)-APT
CON(I,J,K)=CON(I,J,K)+APT*VAR(I,J,K,NVAR)
CP(I,J,K)=(-CP(I,J,K)*VOLW(I,J,K)
& +CIP(I,J,K)+CIM(I,J,K)+CJP(I,J,K)
& +CJM(I,J,K)+CKP(I,J,K)+CKM(I,J,K))/RELAX(NVAR)
CON(I,J,K)=CON(I,J,K)*VOLW(I,J,K)
& +RLAX1*CP(I,J,K)*VAR(I,J,K,NVAR)
DRW(I,J,K)=VOLW(I,J,K)/(ZDG(K)*CP(I,J,K))

205 CONTINUE
RETURN

C ==============================================================================
 ENTRY COEFU
C ==============================================================================

C --- Coefficients for the U equation -----
C
CALL AVGVI
CALL AVGWI

CALL SORU
CALL CFFADD
IF(RELSOR(NVAR).EQ.1.) GO TO 321
RLSOR1 = 1.-RELSOR(NVAR)
DO 320 K=KST,KPT1
DO 320 J=JST,JPT1
DO 320 I=IST,IPT1
  IF(ITER.EQ.0) CONU(I,J,K)=CON(I,J,K)
  CON(I,J,K)=RELSOR(NVAR)*CON(I,J,K)+RLSOR1*CONU(I,J,K)
320  CONU(I,J,K)=CON(I,J,K)
321 CONTINUE
C --- Change UNDERRELAXATION factor ----- 
CALL RELXTN
RLAX1 = 1.-RELAX(NVAR)
C
DO 302 K=KST,KPT1
  DO 302 I=IST,IPT1
    FLOW=VIAVG(I,2,K)*RHOKED(I,2,K)
    DIFF=GAMKED(I,2,K)/YDG(2)
    CALL PWRLAW
    CJM(I,2,K)=CD+DMAX1(0.D0, FLOW)
 302  CJM(I,2,K)=CJM(I,2,K)*RMN(2)*XDSG(I)*ZDF(K)
C
DO 303 J=JST,JPT1
  DO 303 I=IST,IPT1
    FLOW=VIAVG(I,J,2)*RHOJED(I,J,2)
    DIFF=GAMJED(I,J,2)/(R(J)*ZDG(2))
    CALL PWRLAW
    CKM(I,J,2)=CD+DMAX1(0.D0, FLOW)
 303  CKM(I,J,2)=CKM(I,J,2)*YDF(J)*XDSG(I)
C
DO 305 K=KST,KPT1
  DO 305 J=JST,JPT1
    FLOW=U(2,J,K)*RHO(1,J,K)
    DIFF=GAM(1,J,K)/XDF(2)
    CALL PWRLAW
    CIM(3,J,K)=CD+DMAX1(0.D0, FLOW)
    CIM(3,J,K)=CIM(3,J,K)*ARX(J)*ZDF(K)
 305  CIM(I+1,J,K)=CD+DMAX1(0.D0, FLOW)
      IF(I.EQ.IPT1) THEN
        FLOW=U(IPT,J,K)*RHO(IPT,J,K)
        DIFF=GAM(IPT,J,K)/XDF(I)
      ELSE
        FL=U(I,J,K)*RHOIWT(I,J,K)
        FLP=U(I+1,J,K)*RHOIWT(I+1,J,K)
        FLOW=.5*(FL+FLP)
        DIFF=GAM(I,J,K)/XDF(I)
      END IF
    CALL PWRLAW
    CIM(I+1,J,K)=CD+DMAX1(0.D0, FLOW)
    CIM(I,J,K)=CIM(I+1,J,K)-FLOW
    TEMP= ARX(J)*ZDF(K)
    CIM(I,J,K)=CIM(I,J,K)* TEMP
    CIP(I,J,K)=CIP(I,J,K)* TEMP
 303  CIP(I,J,K)=CIP(I,J,K)* TEMP

C
  FLOW=VIAVG(I,J+1,K)*RHOKED(I,J+1,K)
  DIFF=GAMKED(I,J+1,K)/YDG(J+1)
  CALL PWRLAW
  CJM(I,J+1,K)=CD+DMAX1(0.D0, FLOW)
  CJP(I,J,K)=CJM(I,J+1,K)-FLOW
  TEMP= RMN(J+1)*XDSG(I)*ZDF(K)
CJM(I,J+1,K)=CJM(I,J+1,K)* TEMP
CJP(I,J,K)=CJP(I,J,K)* TEMP

FLOW=WI AVG(I,J,K+1)*RHO JED(I,J,K+1)
DIFF=GAM JED(I,J,K+1)/(R(J)*ZDG(K+1))
CALL PWRLAW
CKM(I,J,K+1)=CD+DMAX1(0,DO,FLOW)
CKP(I,J,K)=CKM(I,J,K+1)-FLOW
TEMP=YDF(J)*XDSG(I)
CKM(I,J,K+1)=CKM(I,J,K+1)* TEMP
CKP(I,J,K)=CKP(I,J,K)* TEMP

APT=RHOIWT(I,J,K)/DT
CP(I,J,K)=CP(I,J,K)-APT
CON(I,J,K)=CON(I,J,K)+APT*U(I,J,K)
CP(I,J,K)=(-CP(I,J,K)*VOLU(I,J,K)
& +CIP(I,J,K)+CJM(I,J,K)+CJP(I,J,K)
& +CJM(I,J,K)+CKP(I,J,K)+CKM(I,J,K))/RELAX(NVAR)
& +RLAX*CP(I,J,K)*VAR(I,J,K,NVAR)
DU(I,J,K)=VOLU(I,J,K)/(XDG(I)*CP(I,J,K))

305 CONTINUE
RETURN
C
C ==============================================================
C ENTRY COEFPC
C
C COEFFICIENTS FOR P' EQUATION
C
C CALL RELXTN
C
DO 512 K=KST,KPT1
DO 512 J=JST,JPT1
DO 512 I=IST,IPT1
512 CON(I,J,K)=0.
C
DO 514 K=KST,KPT1
DO 514 I=IST,IPT1
CON(1,2,K)=CON(1,2,K)+RMN(2)*XDF(I)*ZDF(K)*RHO(I,1,K)*V(I,2,K)
CJM(1,2,K)=0.
514 CONTINUE
C
DO 515 J=JST,JPT1
DO 515 I=IST,IPT1
CON(I,J,2)=CON(I,J,2)+YDF(J)*XDF(I)*RHO(I,J,1)*W(I,J,2)
CKM(I,J,2)=0.
515 CONTINUE
C
DO 516 K=KST,KPT1
DO 516 J=JST,JPT1
CON(2,J,K)=CON(2,J,K)+ARX(J)*ZDF(K)*RHO(1,J,K)*U(2,J,K)
CIM(2,J,K)=0.
DO 516 I=IST,IPT1
TEMP=ARX(J)*ZDF(K)*RHOIWT(I+1,J,K)
FLOW = TEMP * U(I+1,J,K)
CON(I,J,K) = CON(I,J,K) - FLOW
IF(I.EQ.IPT1) THEN
  CIP(I,J,K) = 0.
ELSE
  CON(I+1,J,K) = CON(I+1,J,K) + FLOW
  CIP(I,J,K) = TEMP * DU(I+1,J,K)
  CIM(I+1,J,K) = CIP(I,J,K)
END IF

C

TEMP = RMN(J+1) * XDF(I) * ZDF(K) * RHOJWT(I,J+1,K)
FLOW = TEMP * V(I,J+1,K)
CON(I,J,K) = CON(I,J,K) - FLOW
IF(J.EQ.JPT1) THEN
  CJP(I,J,K) = 0.
ELSE
  CON(I,J+1,K) = CON(I,J+1,K) + FLOW
  CJP(I,J,K) = TEMP * DV(I,J+1,K)
  CJM(I,J+1,K) = CJP(I,J,K)
END IF

C

TEMP = YDF(J) * XDF(I) * RHOKWT(I,J,K+1)
FLOW = TEMP * W(I,J,K+1)
CON(I,J,K) = CON(I,J,K) - FLOW
IF(K.EQ.KPT1) THEN
  CKP(I,J,K) = 0.
ELSE
  CON(I,J,K+1) = CON(I,J,K+1) + FLOW
  CKP(I,J,K) = TEMP * DRW(I,J,K+1) / R(J)
  CKM(I,J,K+1) = CKP(I,J,K)
END IF

CP(I,J,K) = CIP(I,J,K) + CIM(I,J,K) + CJP(I,J,K) + CJM(I,J,K)
& + CKP(I,J,K) + CKM(I,J,K)
516 CONTINUE
CALL CFFADD
RETURN

C
C ==---------------------------------------------------------
ENTRY COEFOF
C ==---------------------------------------------------------
C --- Coefficients for the other equations ------
C
CALL GAMMA
CALL PROPWT
IF(NVAR.EQ.NK) THEN
  CALL SOR
  CALL CFFADD
  IF(RELSOR(NVAR).EQ.1.) GO TO 621
  RELSOR1 = 1. - RELSOR(NVAR)
DO 620 K=KST,KPT1
DO 620 J=JST,JPT1
DO 620 I=IST,IPT1
IF(ITER.EQ.0)  CONK(I,J,K) = CON(I,J,K)
CON(I,J,K) = RELSOR(NVAR) * CON(I,J,K)
620 CONTINUE
CALL CFFADD
RETURN
& +RLS0R1*CONK(I,J,K)

CONK(I,J,K)=CON(I,J,K)

CONTINUE

ELSE IF(NVAR.EQ.NK2) THEN
CALL SORK2
CALL CFFADD
IF(RELSOR(NVAR).EQ.1.) GO TO 721
RLS0R1 = 1.-RELSOR(NVAR)
DO 720 K=KST,KPT1
DO 720 J=JST,JPT1
DO 720 I=IST,IPT1
IF(ITER.EQ.0) CONK2(I,J,K)=CON(I,J,K)
CON(I,J,K)=RELSOR(NVAR)*CON(I,J,K)
& +RLS0R1*CONK2(I,J,K)

720 CONK2(I,J,K)=CON(I,J,K)

CONTINUE

END IF
CALL RELXTN
RLAX1 = 1.-RELAX(NVAR)

C

DO 602 K=KST,KPT1
DO 602 I=IST,IPT1
FLOW=V(I,2,K)*RH0(I,1,K)
DIFF=GAM(1,1,K)/YDG(2)
CALL PWRLAW
CJM(1,2,K)=CD+DMAX1(0.D0,FLOW)

602 CJM(I,2,K)=CJM(I,2,K)*RMN(2)*XDF(I)*ZDF(K)

C

DO 603 J=JST,JPT1
DO 603 I=IST,IPT1
FLOW=W(I,J,2)*RH0(I,0,1)
DIFF=GAM(I,J,1)/(R(J)*ZDG(2))
CALL PWRLAW
CKM(I,J,2)=CD+DMAX1(0.D0,FLOW)

603 CKM(I,J,2)=CKM(I,J,2)*YDF(J)*XDF(I)

C

DO 605 K=KST,KPT1
DO 605 J=JST,JPT1
FLOW=U(2,J,K)*RH0(I,J,K)
DIFF=GAM(1,J,K)/XDG(2)
CALL PWRLAW
CIM(2,J,K)=CD+DMAX1(0.D0,FLOW)
CIM(2,J,K)=CIM(2,J,K)*ARX(J)*ZDF(K)

DO 605 I=1ST,IPT1
FLOW=U(I+1,J,K)*RHOIWT(I+1,J,K)
DIFF=GAMIWT(I+1,J,K)/XDG(I+1)
CALL PWRLAW
CIM(I+1,J,K)=CD+DMAX1(0.D0,FLOW)
CIP(I,J,K)=CIM(I+1,J,K)-FLOW
TEMP= ARX(J)*ZDF(K)
CIM(I+1,J,K)=CIM(I+1,J,K)* TEMP
CIP(I,J,K)=CIP(I,J,K)* TEMP

C

FLOW=V(I,J+1,K)*RHOJWT(I,J+1,K)
DIFF = GAMJWT(I,J+1,K)/YDG(J+1)  
CALL PWRLAW  
CJM(I,J+1,K) = CD + DMAX1(0,DO,FLOW)  
CJP(I,J,K) = CJM(I,J+1,K) - FLOW  
TEMP = RMN(J+1)*XDF(I)*ZDF(K)  
CJM(I,J+1,K) = CJM(I,J+1,K) * TEMP  
CJP(I,J,K) = CJP(I,J,K) * TEMP  
C
FLOW = W(I,J,K+1)*RHOKWT(I,J,K+1)  
DIFF = GAMKWT(I,J,K+1)/(R(J)*ZDG(K+1))  
CALL PWRLAW  
CKM(I,J,K+1) = CD + DMAX1(0,DO,FLOW)  
CKP(I,J,K) = CKM(I,J,K+1) - FLOW  
TEMP = YDF(J)*XDF(I)  
CKM(I,J,K+1) = CKM(I,J,K+1) * TEMP  
CKP(I,J,K) = CKP(I,J,K) * TEMP  
C
APT = RHO(I,J,K)/DT  
CP(I,J,K) = CP(I,J,K) - APT  
CON(I,J,K) = CON(I,J,K) + APT*VAR(I,J,K,NVAR)  
CP(I,J,K) = (CP(I,J,K) * VOLM(I,J,K)  
& +CIP(I,J,K)+CIM(I,J,K)+CJP(I,J,K)) / RELAX(NVAR)  
CON(I,J,K) = CON(I,J,K) * VOLM(I,J,K)  
& +RLAX1*CP(I,J,K)*VAR(I,J,K,NVAR)  
605 CONTINUE  
RETURN  
END  
C  
C==================================================================================  
C SUBROUTINE DOMAIN  
C==================================================================================  
C SPECIFY GRID FOR THE CALCULATION DOMAIN  
C  
C IMPLICIT REAL*8 (A-H,O-Z)  
LOGICAL UNIFORM  
COMMON/GRDTYP/UNIFORM  
COMMON/WTING/  
& FX(30),FXM(30),FY(30),FYM(30),FV(30),FVP(30),  
& FZ(30),FZM(30)  
COMMON/SHAPE/ XL,YL,ZL  
COMMON/NPTS/ IPT, IPT1, IPT2, JPT, JPT1, JPT2, KPT, KPT1, KPT2  
COMMON/NODES/  
& X(30), XU(30), XDG(30), XDF(30), XDSG(30),  
& Y(30), YV(30), YDG(30), YDF(30), YDSG(30),  
& Z(30), ZW(30), ZDG(30), ZDF(30), ZDSG(30),  
& YDFR(30), YDSGR(30), ARX(30), ARXJ(30), ARXJP(30),  
& XDFI(30), XDFIP(30), ZDFK(30), ZDFKP(30),  
& R(30), RMN(30), YW(30),  
& VOLM(30,26,25), VOLV(30,26,25),  
& VOLW(30,26,25), VOLU(30,26,25)  
C
ENTRY CFACE
C ==---------------------------------------------------------------------
C C SET CONTROL FACES
C IPT1=IPT-1
IPT2=IPT-2
JPT1=JPT-1
JPT2=JPT-2
KPT1=KPT-1
KPT2=KPT-2
C IF(UNIFORM) THEN
C---- Uniform grid structure -----
DX=XL/FLOAT(IPT2)
XU(2)=0.
1 DO 1 I=3,IPT
1 XU(I)=XU(I-1)+DX
C
DY=YL/FLOAT(JPT2)
YV(2)=0.
2 DO 2 J=3,JPT
2 YV(J)=YV(J-1)+DY
C
DZ=ZL/FLOAT(KPT2)
ZW(2)=0.
3 DO 3 K=3,KPT
3 ZW(K)=ZW(K-1)+DZ
CCC RETURN
C ELSE
C---- Variable grid structure -----
CALL VGRID
END IF
CCC RETURN
C C ==---------------------------------------------------------------------
ENTRY CVOL
C C SET CONTROL VOLUMES (FINITE DOMAINS)
C X(1)=XU(2)
X(IPT)=XU(IPT)
DO 5 I=2,IPT1
5 X(I)=.5*(XU(I+1)+XU(I))
Y(1)=YV(2)
Y(JPT)=YV(JPT)
DO 8 J=2,JPT1
8 Y(J)=.5*(YV(J+1)+YV(J))
Z(1)=ZW(2)
Z(KPT)=ZW(KPT)
DO 10 K=2,KPT1
10 Z(K)=.5*(ZW(K+1)+ZW(K))
DO 12 J=1,JPT
$\text{YW}(J) = Y(J) - Y(JPT)$

$\text{DO } 15 \ I = 2, \text{IPT}$

$XDG(I) = X(I) - X(I-1)$

$\text{DO } 18 \ I = 2, \text{IPT1}$

$XDF(I) = XU(I+1) - XU(I)$

$\text{DO } 20 \ I = 3, \text{IPT1}$

$XDSG(I) = XDG(I)$

$XDSG(3) = XDSG(3) + XDG(2)$

$XDSG(\text{IPT1}) = XDSG(\text{IPT1}) + XDG(\text{IPT})$

$\text{DO } 22 \ I = 3, \text{IPT2}$

$XDFI(I) = 0.5 \times XDF(I)$

$\text{DO } 25 \ J = 2, \text{JPT}$

$YDG(J) = Y(J) - Y(J-1)$

$\text{DO } 30 \ J = 2, \text{JPT1}$

$YDF(J) = YV(J+1) - YV(J)$

$\text{DO } 35 \ J = 3, \text{JPT1}$

$YDSG(J) = YDG(J)$

$YDSG(3) = YDSG(3) + YDG(2)$

$YDSG(\text{JPT1}) = YDSG(\text{JPT1}) + YDG(\text{JPT})$

$\text{DO } 38 \ K = 2, \text{KPT}$

$ZDG(K) = Z(K) - Z(K-1)$

$\text{DO } 40 \ K = 2, \text{KPT1}$

$ZDF(K) = ZW(K+1) - ZW(K)$

$\text{DO } 45 \ K = 3, \text{KPT1}$

$ZDSG(K) = ZDG(K)$

$ZDSG(3) = ZDSG(3) + ZDG(2)$

$ZDSG(\text{KPT1}) = ZDSG(\text{KPT1}) + ZDG(\text{KPT})$

$\text{DO } 47 \ K = 3, \text{KPT2}$

$ZDFK(K) = 0.5 \times ZDF(K)$

$\text{DO } 50 \ J = 2, \text{JPT}$

$R(J) = R(J-1) + YDG(J)$

$\text{RMN}(2) = R(1)$

$\text{RMN}(\text{JPT}) = R(\text{JPT})$

$\text{DO } 55 \ J = 3, \text{JPT1}$

$\text{DO } 62 \ J = 2, \text{JPT1}$

$YDFR(J) = R(J) \times YDF(J)$

$ARX(J) = YDFR(J)$

$\text{CONTINUE}$

$YDSGR(3) = 0.5 \times (R(3) + R(1)) \times YDSG(3)$

$YDSGR(\text{JPT1}) = 0.5 \times (R(\text{JPT}) + R(\text{JPT2})) \times YDSG(\text{JPT1})$

$\text{DO } 64 \ J = 4, \text{JPT2}$

$YDSGR(J) = 0.5 \times (R(J) + R(J-1)) \times YDG(J)$
SUBROUTINE RESIDU

CALCULATE RESIDUES OF TRANSPORT EQUATIONS

IMPLICIT REAL*8 (A-H,O-Z)
COMMON/SUMAX/ CONTOT, CONTMX, RESMAX(14)
COMMON/ITER1/ ITER, LAST, TIME, DT
COMMON/VAR5/ VAR(30,26,25,14)
COMMON/CPN/ CP(30,26,25), CON(30,26,25),
& CIP(30,26,25), CIM(30,26,25),
& CJP(30,26,25), CJM(30,26,25),
& CKP(30,26,25), CKM(30,26,25)
COMMON/NUMBER/
& NVAR, MAXVAR, NW, NZMUT, NGAM, NRH0,
& NV, NRW, NU, NPC, NP, NK, NK2
COMMON/NPTS/ IPT, IPT1, IPT2, JPT, JPT1, JPT2, KPT, KPT1, KPT2
COMMON/FIRST/ IST, JST, KST

IF(NVAR.EQ.NPC) THEN
  CONTMX=0.
  CONTOT=0.
  DO 3300 K=KST, KPT1
       DO 3300 J=JST, JPT1
       DO 3300 I=IST, IPT1
           CONTMX=DMAX1(CONTMX, DABS(CON(I,J,K)))
           CONTOT=CONTOT+CON(I,J,K)
       CONTINUE
  RESMAX(NVAR)=0.
  DO 4300 K=KST, KPT1
       DO 4300 J=JST, JPT1
       DO 4300 I=IST, IPT1
           VALUE= CP(I,J,K)*VAR(I,J,K,NVAR)
           RESDUL= CIP(I,J,K)*VAR(I+1, J, K, NVAR)
           &+CIM(I,J,K)*VAR(I-1, J, K, NVAR)
           &+CJP(I,J,K)*VAR(I, J+1, K, NVAR)
           &+CJM(I,J,K)*VAR(I, J-1, K, NVAR)
           &+CKP(I,J,K)*VAR(I, J, K+1, NVAR)
           &+CKM(I,J,K)*VAR(I, J, K-1, NVAR)
           &+CON(I,J,K)= VALUE
           IF(CP(I,J,K).GE.1.D20) THEN
               RESDUL=RESDUL/CP(I,J,K)
           ELSE IF(VALUE.GE.1.) THEN
               RESDUL=RESDUL/VALUE
           END IF
           RESMAX(NVAR)=DMAX1(RESMAX(NVAR), DABS(RESDUL))
       CONTINUE
   END IF
RETURN
END

C
C============================================================================

SUBROUTINE SWEEPS
C============================================================================

C TDMA WITH SWEEP METHOD
C

IMPLICIT REAL*8 (A-H,O-Z)
COMMON/VARS/ VAR(30,26,25,14)
COMMON/CALN/ CP(30,26,25),CON(30,26,25),
&    CIP(30,26,25),CIM(30,26,25),
&    CJP(30,26,25),CJM(30,26,25),
&    CKP(30,26,25),CKM(30,26,25)
COMMON/NUMBER/
&      NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
&      NV,NRW,NU,NPC,NP,NK,NK2
COMMON/NSWEEP/ NISP,NJSP,NKSP
COMMON/NPTS/ IPT,IPT1,IPT2,JPT,JPT1,JPT2,KPT,KPT1,KPT2
COMMON/FIRST/ IST,JST,KST
COMMON/FIRST1/ IST1,JST1,KST1
COMMON/NTIME1/ NTIMES(14)

C
IST1 = IST - 1
JST1 = JST - 1
KST1 = KST - 1
DO 501 NT=1,NTIMES(NVAR)
   DO 190 K=KST,KPT1
      DO 170 JSP=1,NJSP
         JLAST=JPT1
         IF(MOD(JSP,2).EQ.O) JLAST=JPT2
         DO 170 JJ=JST,JLAST
            J=JJ
            IF(MOD(JSP,2).EQ.O) J=JST+JLAST-JJ
            CALL TDMAI(J,K)
      170 CONTINUE
190 CONTINUE
   DO 290 I=IST,IPT1
      DO 270 KSP=1,NKSP
         KLAST=KPT1
         IF(MOD(KSP,2).EQ.O) KLAST=KPT2
         DO 270 KK=KST,KLAST
            K=KK
            IF(MOD(KSP,2).EQ.O) K=KST+KLAST-KK
            CALL TDMAJ(K,I)
      270 CONTINUE
290 CONTINUE
   DO 390 J=JST,JPT1
      DO 370 ISP=1,NISP
         ILAST=IPT1
         IF(MOD(ISP,2).EQ.O) ILAST=IPT2
         DO 370 II=IST,ILAST
            I=II
            IF(MOD(ISP,2).EQ.O) I=IST+ILAST-II
            CALL TDMAK(I,J)
      370 CONTINUE
390 CONTINUE
```fortran
370 CONTINUE
390 CONTINUE
501 CONTINUE
RETURN
END

C
C=====================================================================
SUBROUTINE TDMAD3
C=====================================================================

C TRI-DIAGONAL MATRIX ALGORITHM IN 3D

IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION AA(50),BB(50)
COMMON/VARS/ VAR(30,26,25,14)
COMMON/CAHN/ CP(30,26,25), CON(30,26,25),
& CIP(30,26,25), CIM(30,26,25),
& CJP(30,26,25), CJM(30,26,25),
& CKP(30,26,25), CKM(30,26,25)
COMMON/NUMBER/
& NVAR, MAXVAR, NW, NZMUT, NGAM, NRHO,
& NV, NRW, NU, NPC, NP, NK, NK2
COMMON/NPTS/ IPT, IPT1, IPT2, JPT, JPT1, JPT2, KPT, KPT1, KPT2
COMMON/FIRST/ IST, JST, KST
COMMON/FIRST1/ IST1, JST1, KST1

C
C=====================================================================
ENTRY TDMAI(J,K)
C=====================================================================

C TDMA IN I-DIRECTION

C AA(IST1)=0.
BB(IST1)=VAR(IST1,J,K,NVAR)
DO 130 ID=IST, IPT1
   DENOM=CP(ID,J,K)-AA(ID-1)*CIM(ID,J,K)
   AA(ID)=CIP(ID,J,K)/DENOM
   IF(DENOM.GT.1.D20) THEN
      AA(ID)=0.
      BB(ID)=CON(ID,J,K)/CP(ID,J,K)
   ELSE
      TEMP=CON(ID,J,K)+CJP(ID,J,K)*VAR(ID,J+1,K,NVAR)
&      +CJM(ID,J,K)*VAR(ID,J-1,K,NVAR)
&      +CKP(ID,J,K)*VAR(ID,J,K+1,NVAR)
&      +CKM(ID,J,K)*VAR(ID,J,K-1,NVAR)
      BB(ID)=(TEMP+CIM(ID,J,K)*BB(ID-1))/DENOM
   END IF
130 CONTINUE
DO 150 II=IST, IPT1
   ID=IST+IPT1-II
   VAR(ID,J,K,NVAR)=VAR(ID+1,J,K,NVAR)*AA(ID)+BB(ID)
150 RETURN

C
C=====================================================================
```
VAR(I,J,K,VAR)=VAR(I,J+1,K,VAR)+VAR(I,J,K,VAR)
END IF

320 CONTINUE

DO 320 K=ISTI,KPI1

330 CONTINUE

END

RETURN

DO 320 K=ISTI,KPI1

350 CONTINUE

BB(AK0)=(TEM+CMW(I,J,K)+VAR(I,J,K)+VAR(I,J,K,VAR)+VAR(I,J,K,VAR)+VAR(I,J,K,VAR))

ELSE

BB(AK0)=0.

IF (DENM(0,J,20)+CMW(I,J,K)+VAR(I,J,K)+VAR(I,J,K,VAR)+VAR(I,J,K,VAR)) IJ

BB(20)=CMW(I,J,K)+CMW(I,J,K)+VAR(I,J,K)+VAR(I,J,K,VAR)

260 CONTINUE

308 CONTINUE

END IF

RETURN

VAR(I,J,K,VAR)=VAR(I,J+1,K,VAR)+VAR(I,J,K,VAR)

ENTRY TOMAK(I,J)

ENTRY TOMAK(I,J)

ENTRY TOMAK(I,J)
SUBROUTINE PWRLAW

C ==================================================================
C POWER LAW SCHEME
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/PWRL/FLOW,DIF,F,D
D=DIF
IF(FLOW.EQ.0.) RETURN
TEMP=DIF- DABS(FLOW)*0.1
D=0.
IF(TEMP.LE.0.) RETURN
TEMP=TEMP/DIF
D=DIF*TEMP**5
RETURN
END

C ===========

SUBROUTINE GAMMA

C ==================================================================
C CALCULATE EXCHANGE COEFFICIENTS
C
IMPLICIT REAL*8 (A-H,O-Z)
LOGICAL NOTURB,ONCE
DIMENSION GAMOLD(30,26,25)
COMMON/GAM2/ NOTURB,ONCE
COMMON/SOLVST/ NSOLST
COMMON/LAXVAR/ RELAX(14)
COMMON/VARS/ VAR(30,26,25,14)
COMMON/NUMBER/
& NVAR, MAXVAR, NW, NZMUT, NGAM, NRHO,
& NV, NRW, NU, NPC, NP, NK, NK2
COMMON/ITER1/ ITER, LAST, TIME, DT
COMMON/NPTS/ IPT, IPT1, IPT2, JPT, JPT1, JPT2, KPT, KPT1, KPT2
COMMON/GAMLAM/ ZMUL
DIMENSION U(30,26,25), V(30,26,25), PC(30,26,25), P(30,26,25),
& RW(30,26,25), W(30,26,25), ZK(30,26,25), ZK2(30,26,25),
& ZMUT(30,26,25), GAM(30,26,25), RHO(30,26,25)
EQUIVALENCE
& (VAR(1,1,1,1), V(1,1,1)) , (VAR(1,1,1,2), RW(1,1,1)),
& (VAR(1,1,1,3), U(1,1,1)),
& (VAR(1,1,1,4), P(1,1,1)) , (VAR(1,1,1,5), PC(1,1,1)),
& (VAR(1,1,1,6), ZK(1,1,1)) , (VAR(1,1,1,7), ZK2(1,1,1))
EQUIVALENCE
& (VAR(1,1,1,11), W(1,1,1)) , (VAR(1,1,1,12), ZMUT(1,1,1)),
& (VAR(1,1,1,13), GAM(1,1,1)) , (VAR(1,1,1,14), RHO(1,1,1))
C
C3D IF(ONCE) THEN
C DO 1100 K=1,KPT
C DO 1100 J=1,JPT
C DO 1100 I=1,IPT
C1100 ZMUT(I,J,K)=0.
C ONCE=.FALSE.
C3D END IF
C
IF(NVAR.NE.NSOLST) GO TO 1201
IF(.NOT.NOTURB) CALL TURB
1201 CALL GAMFAC(RATIO)
DO 1300 K=1,KPT
DO 1300 J=1,JPT
DO 1300 I=1,IPT
GAM(I,J,K)=(ZMUL+ZMUT(I,J,K))/RATIO
1300 CONTINUE
IF(RELAX(NGAM).EQ.1.) RETURN
RLAX1= 1.-RELAX(NGAM)
DO 1400 K=1,KPT
DO 1400 J=1,JPT
DO 1400 I=1,IPT
IF(ITER.EQ.0) GAMOLD(I,J,K)=GAM(I,J,K)
C -------- To avoid underflow ---------------------
IF(GAM(I,J,K).LT.1.D-30) GAM(I,J,K)=0.
GAM(I,J,K)=RELAX(NGAM)*GAM(I,J,K) + RLAX1*GAMOLD(I,J,K)
1400 GAMOLD(I,J,K)=GAM(I,J,K)
C RETURN
END
C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
SUBROUTINE RELXTN
C CHANGE RELAXATION FACTORS
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/NUMBER/
& NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
& NV,NRW,NP,NPC,NP,NK,NK2
COMMON/ITER1/ ITER,LAST,TIME,DT
COMMON/LAXVAR/ RELAX(14)
COMMON/LAX2/ ITRLAX(9),NCHNGE(14)
COMMON/LAX3/ DBETA(9,14)
C
IF(NCHNGE(NVAR).EQ.0) RETURN
IF(RELAX(NVAR).GE.0.9) RETURN
NX=NVAR
IF(NVAR.EQ.NPC) NX= NP
C
NTEMP=NCHNGE(NX)
DO 1818 I=1,NTEMP
IF(ITER.EQ.ITRLAX(I)) RELAX(NX)=RELAX(NX)+DBETA(I,NX)
1818 CONTINUE
C RETURN
END
C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
SUBROUTINE PHIAVG
C
C INTERPOLATE VARIABLES
C
IMPLICIT REAL*8 (A-H,O-Z)
LOGICAL RHOVAR
COMMON/RH0V/RH0VAR
COMMON/VARS/ VAR(30,26,25,14)
COMMON/VELAVG/ UJAVG(30,26,25),VIAVG(30,26,25),WIAVG(30,26,25),
& UKAVG(30,26,25),VKAvg(30,26,25),WJAVG(30,26,25),
& COMMON/PROP/RHOIWT(30,26,25),RHOJWT(30,26,25),RHOKWT(30,26,25),
& GAMIWT(30,26,25),GAMJWT(30,26,25),GAMKWT(30,26,25),
& RHOIED(30,26,25),RHOJED(30,26,25),RHOKED(30,26,25),
& GAMIED(30,26,25),GAMJED(30,26,25),GAMKED(30,26,25)
COMMON/NODES/
& X(30),XU(30),XDG(30),XDF(30),XDSG(30),
& Y(30),YV(30),YDG(30),YDF(30),YDSG(30),
& Z(30),Zw(30),ZDG(30),ZDF(30),ZDSG(30),
& YDFR(30),YDSR(30),ARX(30),ARXJ(30),ARXJP(30),
& XDFI(30),XDFIP(30),ZDFK(30),ZDFKP(30),
& R(30),RMN(30),YW(30),
& VOLM(30,26,25), V0LV(30,26,25),
& VOLW(30,26,25),VOLU(30,26,25)
COMMON/WTING/
& FX(30),FXM(30),FY(30),FYM(30),FV(30),FVP(30),
& FZ(30),FZM(30)
COMMON/NUMBER/
& NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
& NV,NRW,NU,NPC,NP,NK,NK2
COMMON/ITER1/ ITER,LAST,TIME,DT
COMMON/NPTS/ IPT,IPT1,IPT2,JPT,JPT1,JPT2,KPT,KPT1,KPT2
COMMON/FIRST/ IST,JST,KST
COMMON/OVERFL/ OVFLW
DIMENSION U(30,26,25),V(30,26,25),PC(30,26,25),P(30,26,25),
& RW(30,26,25),W(30,26,25),ZK(30,26,25),ZK2(30,26,25),
& ZMUT(30,26,25),GAM(30,26,25),RHO(30,26,25)
EQUIVALENCE
& (VAR(1,1,1,1),U(1,1,1)),(VAR(1,1,1,2),RW(1,1,1)),
& (VAR(1,1,1,3),U(1,1,1)),
& (VAR(1,1,1,4),P(1,1,1)),(VAR(1,1,1,5),PC(1,1,1)),
& (VAR(1,1,1,6),ZK(1,1,1)),(VAR(1,1,1,7),ZK2(1,1,1))
EQUIVALENCE
& (VAR(1,1,1,11),W(1,1,1)),(VAR(1,1,1,12),ZMUT(1,1,1)),
& (VAR(1,1,1,13),GAM(1,1,1)),(VAR(1,1,1,14),RHO(1,1,1))
C
C ENTRY PROPWT
C
C FOR DENSITY AND EXCHANGE COEFFICIENTS
C
DO 4100 K=1,KPT
DO 4100 J=1,JPT
DO 4100 I=2,IPT
IF(ITER.EQ.0.OR.RHOVAR)
& RHOJWT(I,J,K)=FXM(I)*RHO(I-1,J,K)+FX(I)*RHO(I,J,K)
& GAMIJWT(I,J,K)=1/(FXM(I)/(GAM(I,J,K)+OVFLW)
& +FX(I)/(GAM(I-1,J,K)+OVFLW))
IF(I.EQ.2) GAMIWT(2,J,K)=GAM(1,J,K)
IF(I.EQ.IPT) GAMIWT(IPT,J,K)=GAM(IPT,J,K)
4100 CONTINUE
C
DO 4150 K=1,KPT
DO 4150 I=1,IPT
DO 4150 J=2,JPT
IF(ITER.EQ.0.OR.RHOVAR)
& RHOJWT(I,J,K)=FYM(J)*RHO(I,J-1,K)+FY(J)*RHO(I,J,K)
& GAMJWT(I,J,K)=1/(RMN(J)*FYM(J)/(R(J)*GAM(I,J,K)+OVFLW)
& +FY(J)/(R(J-1)*GAM(I,J-1,K)+OVFLW)+OVFLW)
IF(J.EQ.2) GAMJWT(1,2,K)=GAM(I,1,K)
IF(J.EQ.JPT) GAMJWT(I,JPT,K)=GAM(I,JPT,K)
4150 CONTINUE
C
DO 4200 J=1,JPT
DO 4200 I=1,IPT
DO 4200 K=2,KPT
IF(ITER.EQ.0.OR.RHOVAR)
& RHOJWT(I,J,K)=FZM(K)*RHO(I,J,K-1)+FZ(K)*RHO(I,J,K)
& GAMJWT(I,J,K)=1/(FZM(K)/(GAM(I,J,K)+OVFLW)
& +FZ(K)/(GAM(I,J,K-1)+OVFLW))
IF(K.EQ.2) GAMJWT(I,J,2)=GAM(I,J,1)
IF(K.EQ.KPT) GAMJWT(I,J,KPT)=GAM(I,J,KPT)
4200 CONTINUE
C
DO 4300 K=2,KPT
DO 4300 I=2,IPT
DO 4300 J=2,JPT
IF(ITER.EQ.0.OR.RHOVAR)
& RHOJWT(I,J,K)=FZM(K)*RHO(I,J,K-1)+FZ(K)*RHO(I,J,K)
& GAMJWT(I,J,K)=1/(FZM(K)/(GAM(I,J,K)+OVFLW)
& +FZ(K)/(GAM(I,J,K-1)+OVFLW))
IF(K.EQ.2) GAMJWT(I,J,2)=GAM(I,J,1)
IF(K.EQ.KPT) GAMJWT(I,J,KPT)=GAM(I,J,KPT)
4300 CONTINUE
C
DO 4350 I=2,IPT
DO 4350 K=2,KPT
DO 4350 J=2,JPT
IF(ITER.EQ.0.OR.RHOVAR)
& RHOJWT(I,J,K)=FXM(I)*RHO(I-1,J,K)+FX(I)*RHO(I,J,K)
& GAMJWT(I,J,K)=1/(FXM(I)/(GAM(I,J,K)+OVFLW)
& +FX(I)/(GAM(I-1,J,K)+OVFLW))
IF(I.EQ.2) GAMJWT(2,J,K)=GAMKWT(1,J,K)
IF(I.EQ.IPT) GAMJWT(IPT,J,K)=GAMKWT(IPT,J,K)
4350 CONTINUE
C
DO 4400 J=2,JPT
DO 4400 I=2,IPT
DO 4400 K=2,KPT
IF(ITER.EQ.0.OR.RHOVAR)
& RHOKE(I,J,K)=FYM(J)*RHOIWT(I,J-1,K)+FY(J)*RHOIWT(I,J,K)
GAMKE(I,J,K)=1/(RMN(J)*(FYM(J)/(R(J)*GAMIWT(I,J,K)+OVFLW)
& +FY(J)/(R(J-1)*GAMIWT(I,J-1,K)+OVFLW))+OVFLW)
IF(J.EQ.2) GAMKE(I,2,K)=GAMIWT(I,1,K)
IF(J.EQ.JPT) GAMKE(I,JPT,K)=GAMIWT(I,JPT,K)
4400 CONTINUE
RETURN
C
C =====================================================

ENTRY AVGK
C
C FOR VELOCITIES
C
DO 4600 J=2,JPT
DO 4600 I=2,IPT
VKAVG(I,J,2)=V(I,J,1)
VKAVG(I,J,KPT)=V(I,J,KPT)
DO 4600 K=3,KPT1
FL=ZDFK(K)*V(I,J,K)*RHOJWT(I,J,K)
FLM=ZDFKP(K-1)*V(I,J,K-1)*RHOJWT(I,J,K-1)
VKAVG(I,J,K)=(FL+FLM)/(ZDSG(K)*RHOIWE(I,J,K))
4600 CONTINUE
RETURN
C
C =====================================================

ENTRY AVGUK
C
DO 4650 J=2,JPT
DO 4650 I=2,IPT
UKAVG(I,J,2)=U(I,J,1)
UKAVG(I,J,KPT)=U(I,J,KPT)
DO 4650 K=3,KPT1
FL=ZDFK(K)*U(I,J,K)*RHOIWT(I,J,K)
FLM=ZDFKP(K-1)*U(I,J,K-1)*RHOIWT(I,J,K-1)
UKAVG(I,J,K)=(FL+FLM)/(ZDSG(K)*RHOIWE(I,J,K))
4650 CONTINUE
RETURN
C
C =====================================================

ENTRY AVGJ
C
DO 4700 K=2,KPT
DO 4700 I=2,IPT
WJAVG(I,2,K)=W(I,1,K)
WJAVG(I,JPT,K)=W(I,JPT,K)
DO 4700 J=3,JPT1
FL=ARXJ(J)*W(I,J,K)*RHOJWT(I,J,K)
FLM=ARXJP(J-1)*W(I,J-1,K)*RHOJWT(I,J-1,K)
WJAVG(I,J,K)=(FL+FLM)/(YDSGR(J)*RHOIWE(I,J,K))
4700 CONTINUE
RETURN
C
C  ====================================================
C  ENTRY AVGUJ
C  ====================================================
C
DO 4750 K=2,KPT
DO 4750 I=2,IPT
   UJAVG(I,2,K)=U(I,1,K)
   UJAVG(I,JPT,K)=U(I,JPT,K)
DO 4750 J=3,JP1
   FL=ARXJ(J)*U(I,J,K)*RHOIWT(I,J,K)
   FLM=ARXJP(J-1)*U(I,J-1,K)*RHOIWT(I,J-1,K)
   UJAVG(I,J,K)=(FL+FLM)/(YDSGR(J)*RHOJED(I,J,K))
4750 CONTINUE
RETURN
C
C  ====================================================
C  ENTRY AVGVI
C  ====================================================
C
DO 4800 K=2,KPT
DO 4800 J=2,JPT
   VIAVG(2,J,K)=V(I,J,K)
   VIAVG(IPT,J,K)=V(IPT,J,K)
DO 4800 I=3,IP1
   FL=XDFI(I)*V(I,J,K)*RHOJWT(I,J,K)
   FLM=XDFIP(I-1)*V(I-1,J,K)*RHOJWT(I-1,J,K)
   VIAVG(I,J,K)=(FL+FLM)/(XDSG(I)*RHOJED(I,J,K))
4800 CONTINUE
RETURN
C
C  ====================================================
C  ENTRY AVGWI
C  ====================================================
C
DO 4850 K=2,KPT
DO 4850 J=2,JPT
   WIAVG(2,J,K)=W(I,J,K)
   WIAVG(IPT,J,K)=W(IPT,J,K)
DO 4850 I=3,IP1
   FL=XDFI(I)*W(I,J,K)*RHOKWT(I,J,K)
   FLM=XDFIP(I-1)*W(I-1,J,K)*RHOKWT(I-1,J,K)
   WIAVG(I,J,K)=(FL+FLM)/(XDSG(I)*RHOKED(I,J,K))
4850 CONTINUE
RETURN
C
END
C
C  ====================================================
C  SUBROUTINE SOURCE
C  ====================================================
C
A SUBROUTINE FOR THE SOURCE TERMS IN ISOTROPIC MODEL.
COMPARABLE TO SUBROUTINE SOURCN FOR NONISOTROPIC MODEL
C SOURCE AND SOURCEN SHOULD NOT BE IN THIS PROGRAM AT THE SAME TIME.

C

IMPLICIT REAL*8 (A-H,O-Z)
COMMON/VARS/ VAR(30,26,25,14)
COMMON/CALN/ CP(30,26,25),CON(30,26,25),
& CIP(30,26,25),CIM(30,26,25),
& CJP(30,26,25),CJM(30,26,25),
& CKP(30,26,25),CKM(30,26,25)
COMMON/VELAVG/ UJAVG(30,26,25),VIAVG(30,26,25),WIAVG(30,26,25),
& UKAVG(30,26,25),VKAvg(30,26,25),WJAVG(30,26,25)
COMMON/PROP/RHOIWT(30,26,25),RHOJW(30,26,25),RHOJW(30,26,25),
& GAMIWT(30,26,25),GAMJW(30,26,25),GAMKJW(30,26,25),
& RHOED(30,26,25),RHOJED(30,26,25),RHOKED(30,26,25),
& GAME(30,26,25),GAMJED(30,26,25),GAMKED(30,26,25)
COMMON/NODES/
& X(30),XU(30),XDG(30),XDF(30),XDSG(30),
& Y(30),YV(30),YDG(30),YDF(30),YDSG(30),
& Z(30),ZW(30),ZDG(30),ZDF(30),ZDSG(30),
& YDFR(30),YDSGR(30),ARX(30),ARXJ(30),ARXJP(30),
& XDFI(30),XDFIP(30),ZDFK(30),ZDFKP(30),
& R(30),RMN(30),YW(30),
& VOLM(30,26,25),VOLV(30,26,25),
& VOLW(30,26,25),VOLU(30,26,25)
COMMON/WTING/
& FX(30),FXM(30),FY(30),FYM(30),FV(30),FVP(30),
& FZ(30),FZM(30)
COMMON/NUMBER/
& NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
& NV,NRW,NU,NPC,NN,NK,NK2
COMMON/ITER1/ ITER,LAST,TIME,DT
COMMON/NPTS/ IPT,IP1,IP2,JPT,JPT1,JPT2,KPT,KPT1,KPT2
COMMON/FIRST/ IST,JST,KST
COMMON/GAMLAM/ ZMUL
COMMON/SOR1/ GZ,GCG,PATM
COMMON/OVERFL/ OVFLW
COMMON/SORTUR/ CMU(30,26,25),RT(30,26,25)
COMMON/LAXDT/ DTLAX(14)
DIMENSION GI(30,26,25)
DIMENSION DWDR(30,26,25),WR(30,26,25)
DIMENSION U(30,26,25),V(30,26,25),PC(30,26,25),P(30,26,25),
& RW(30,26,25),W(30,26,25),ZK(30,26,25),ZK2(30,26,25),
& ZMUT(30,26,25),GAM(30,26,25),RHO(30,26,25)
EQUIVALENCE
& (VAR(1,1,1,1),V(1,1,1)),(VAR(1,1,1,2),RW(1,1,1)),
& (VAR(1,1,1,3),U(1,1,1)),
& (VAR(1,1,1,4),P(1,1,1)),(VAR(1,1,1,5),PC(1,1,1)),
& (VAR(1,1,1,6),ZK(1,1,1)),(VAR(1,1,1,7),ZK2(1,1,1))
EQUIVALENCE
& (VAR(1,1,1,11),W(1,1,1)),(VAR(1,1,1,12),ZMUT(1,1,1)),
& (VAR(1,1,1,13),GAM(1,1,1)),(VAR(1,1,1,14),RHO(1,1,1))
C SOURCE TERM FOR V
C
DO 2100 K=KST,KPT1
DO 2100 J=JST,JPT1
DO 2100 I=IST,IPT1

TEMP= 0.5* (WJAVG(I,J,K)+WJAVG(I,J,K+1))
CON(I,J,K)= RHOJW(I,J,K)*TEMP**2/RMN(J)

TEMP31=R(J)*GAM(I,J,K)/YDF(J)
TEMP32=R(J-1)*GAM(I,J-1,K)/YDF(J-1)
IF(J.EQ.JST) THEN
TEMP32=R(1)*GAM(1,1,K)/YDF(J-1)
ELSE IF(J.EQ.JPT1) THEN
TEMP31=R(JPT)*GAM(I,JPT,K)/YDF(J)
END IF
TEMP=TEMP31*V(I,J+1,K)+TEMP32*V(I,J-1,K)

TEMP3=TEMP31*V(I,J+1,K)+TEMP32*V(I,J-1,K)

IF(J.EQ.JST) THEN
TEMP41=(W(I,J,K+1)-W(I,1,K+1))/YDSG(J)
TEMP42=(W(I,J,K)-W(I,1,K))/YDSG(J)
ELSE IF(J.EQ.JPT1) THEN
TEMP41=(W(I,JPT,K+1)-W(I,J-l,K+1))/YDSG(J)
TEMP42=(W(I,JPT,K)-W(I,J-l,K))/YDSG(J)
ELSE
TEMP41=(W(I,J,K+1)-W(I,J-l,K+1))/YDSG(J)
TEMP42=(W(I,J,K)-W(I,J-l,K))/YDSG(J)
END IF

TEMP41=GAMIED(I,J,K+1)* ( TEMP41-WJAVG(I,J,K+1)/RMN(J) )
TEMP42=GAMIED(I,J,K)* ( TEMP42-WJAVG(I,J,K)/RMN(J) )

IF(J.EQ.JST) THEN
IF(I.EQ.IST) TEMP51=GAMKED(I,J,K)*(U(I,J,K)-U(I,1,K))/YDSG(J)
TEMP52=TEMP51
TEMP51=GAMKED(I+1,J,K)*(U(I+1,J,K)-U(I+1,1,K))/YDSG(J)
ELSE IF(J.EQ.JPT1) THEN
IF(I.EQ.IST) &
TEMP51=GAMKED(I,J,K)*(U(I,JPT,K)-U(I,J-1,K))/YDSG(J)
TEMP52=TEMP51
TEMP51=GAMKED(I+1,J,K)*(U(I+1,JPT,K)-U(I+1,J-1,K))/YDSG(J)
ELSE
TEMP51=GAMKED(I+1,J,K)*(U(I+1,J,K)-U(I+1,J-1,K))/YDSG(J)
TEMP52=TEMP51
TEMP51=GAMKED(I+1,J,K)*(U(I+1,J,K)-U(I+1,J-1,K))/YDSG(J)
END IF

CON(I,J,K)=CON(I,J,K)+(TEMP51-TEMP52)/XDF(I)

C
TEMP6= (WJAVG(I,J,K+1)-WJAVG(I,J,K))/ZDF(K)
CON(I,J,K)=CON(I,J,K)-2.*GAMJWT(I,J,K)/RMN(J)**2

C
CP(I,J,K)=CP(I,J,K) - 2.*GAMJWT(I,J,K)/RMN(J)**2

2100 CONTINUE
RETURN
C
C =============================================================
ENTRY SORRW
C =============================================================
C C SOURCE TERM FOR RW
C
DO 2200 K=KST,KPT1
DO 2200 J=JST,JPT1
DO 2200 I=IST,IPT1
TEMP2 = 2./YDFR(J)
IF(J.EQ.2 .OR. J.EQ.JPT1) THEN
   CP(I,J,K) = 0.
   TEMP = GAMIED(I,J+1,K)*RMN(J+1)*WJAVG(I,J+1,K)
   & -GAMIED(I,J,K)*RMN(J)*WJAVG(I,J,K)
   CON(I,J,K) = -TEMP2*TEMP
ELSE
   TEMP = GAMIED(I,J+1,K)*RMN(J+1)/YDSGR(J+1)
   CP(I,J,K) = -TEMP2*TEMP*ARXJP(J)
   TEMP = TEMP*ARXJ(J+1)*W(I,J+1,K)
   & -GAMIED(I,J,K)*RMN(J)*WJAVG(I,J,K)
   CON(I,J,K) = -TEMP2*TEMP
END IF
C
IF(K.EQ.KST) THEN
   TEMP31 = (V(I,J+1,K)-V(I,J+1,1))/ZDSG(K)
   TEMP32 = (V(I,J,K)-V(I,J,1))/ZDSG(K)
ELSE IF(K.EQ.KPT1) THEN
   TEMP31 = (V(I,J+1,KPT)-V(I,J+1,K-1))/ZDSG(K)
   TEMP32 = (V(I,J,KPT)-V(I,J,K-1))/ZDSG(K)
ELSE
   TEMP31 = (V(I,J+1,K)-V(I,J+1,K-1))/ZDSG(K)
   TEMP32 = (V(I,J,K)-V(I,J,K-1))/ZDSG(K)
END IF
TEMP31 = RMN(J+1)*GAMIED(I,J+1,K)*TEMP31
TEMP32 = RMN(J)*GAMIED(I,J,K)*TEMP32
CON(I,J,K) = CON(I,J,K) + (TEMP31 - TEMP32)/YDFR(J)
C
TEMP41 = GAM(I,J,K)/ZDF(K)
TEMP42 = GAM(I,J,K-1)/ZDF(K-1)
IF(K.EQ.KST) THEN
   TEMP42 = GAM(I,J,1)/ZDF(K-1)
ELSE IF(K.EQ.KPT1) THEN
   TEMP41 = GAM(I,J,KPT)/ZDF(K)
END IF
TEMP4 = TEMP41*RW(I,J,K+1)+TEMP42*RW(I,J,K-1)
TEMP = R(J)**2*ZDSG(K)
CON(I,J,K) = CON(I,J,K) + TEMP4/TEMP
CP(I,J,K) = CP(I,J,K) - (TEMP41 + TEMP42)/TEMP
C
TEMP51 = 0.5*GAM(I,J,K)*(V(I,J+1,K)+V(I,J,K))
TEMP52 = 0.5*GAM(I,J,K-1)*(V(I,J+1,K-1)+V(I,J,K-1))
IF(K.EQ.KST) THEN
   TEMP52 = 0.5*GAM(I,J,1)*(V(I,J+1,1)+V(I,J,1))
ELSE IF(K.EQ.KPT1) THEN
  TEMP51=0.5*GAM(I,J,KPT)*(V(I,J+1,KPT)+V(I,J,KPT))
END IF
CON(I,J,K)=CON(I,J,K)+2.*(TEMP51-TEMP52)/(R(J)*ZDSG(K))

C
IF(K.EQ.KST) THEN
  IF(I.EQ.1ST) TEMP61=(U(I,J,K)-U(I,J,1))/ZDSG(K)
  TEMP62=TEMP61
  TEMP61=(U(I+1,J,K)-U(I+1,J,1))/ZDSG(K)
ELSE IF(K.EQ.KPT1) THEN
  IF(I.EQ.1ST) TEMP61=(U(I,J,KPT)-U(I,J,K-1))/2DSG(K)
  TEMP62=TEMP61
  TEMP61=(U(I+1,J,KPT)-U(I+1,J,K-1))/ZDSG(K)
ELSE
  IF(I.EQ.1ST) TEMP61=(U(I,J,K)-U(I,J,K-1))/ZDSG(K)
  TEMP62=TEMP61
  TEMP61=(U(I+1,J,K)-U(I+1,J,K-1))/ZDSG(K)
END IF
  TEMP61=GAMJED(I+1,J,K)*TEMP61
  TEMP62=GAMJED(I,J,K)*TEMP62
  CON(I,J,K)=CON(I,J,K)+(TEMP61-TEMP62)/XDF(I)
2200 CONTINUE
RETURN
C
C=====================================================================
ENTRY SOUR
C=====================================================================
C
C SOURCE TERM FOR U
C
DO 2300 K=KST,KPT1
DO 2300 J=JST,JPT1
DO 2300 I=1ST,IPT1
  CON(I,J,K)= RHOIWT(I,J,K)*GZ/GC
C
IF(I.EQ.1ST) THEN
  TEMP31=(V(I,J+1,K)-V(1,J+1,K))/XDSG(I)
  TEMP32=(V(I,J,K)-V(1,J,K))/XDSG(I)
ELSE IF(I.EQ.IPT1) THEN
  TEMP31=(V(IPT,J+1,K)-V(I-1,J+1,K))/XDSG(I)
  TEMP32=(V(IPT,J,K)-V(I-1,J,K))/XDSG(I)
ELSE
  TEMP31=(V(I,J+1,K)-V(I-1,J+1,K))/XDSG(I)
  TEMP32=(V(I,J,K)-V(I-1,J,K))/XDSG(I)
END IF
  TEMP31=RMN(J+1)*GAMKED(I,J+1,K)*TEMP31
  TEMP32=RMN(J)*GAMKED(I,J,K)*TEMP32
  CON(I,J,K)=CON(I,J,K)+(TEMP31-TEMP32)/YDFR(J)
C
IF(I.EQ.1ST) THEN
  TEMP41=(W(I,J,K+1)-W(1,J,K+1))/XDSG(I)
  TEMP42=(W(I,J,K)-W(1,J,K))/XDSG(I)
ELSE IF(I.EQ.IPT1) THEN
  TEMP41=(W(IPT,J,K+1)-W(I-1,J,K+1))/XDSG(I)
  TEMP42=(W(IPT,J,K)-W(I-1,J,K))/XDSG(I)
ELSE
    TEMP41=(W(I,J,K+1)-W(I-1,J,K+1))/XDSG(I)
    TEMP42=(W(I,J,K)-W(I-1,J,K))/XDSG(I)
END IF
    TEMP41=GAMJED(I,J,K+1)*TEMP41
    TEMP42=GAMJED(I,J,K)*TEMP42
    CON(I,J,K)=CON(I,J,K)+(TEMP41-TEMP42)/(R(J)*ZDF(K))

    TEMP51=GAM(I,J,K)/XDF(I)
    TEMP52=GAM(I-1,J,K)/XDF(I-1)
    IF(I.EQ.IST) THEN
        TEMP52=GAM(I,J,K)/XDF(I-1)
    ELSE IF(I.EQ.IPT1) THEN
        TEMP51=GAM(IPT,J,K)/XDF(I)
    END IF
    TEMP5=TEMP51*U(I+1,J,K)+TEMP52*U(I-1,J,K)
    CON(I,J,K)=CON(I,J,K)+TEMP5/XDSG(I)
    CP(I,J,K)=-((TEMP51+TEMP52)/XDSG(I))
    CONTINUE
    RETURN

ENTRY SORK

SOURCE TERM FOR K

CALL AVGWJ
CALL AVGUJ
CALL AVGVK
CALL AVGUK
CALL AVGWI
DO 2600 K=KST,KPT1
DO 2600 J=JST,JPT1
DO 2600 I=IST,IPT1
    DVDR=(V(I,J+1,K)-V(I,J,K))/YDF(J)
    IF(DABS(DVDR).GE.1.E-10) THEN
        TEMP1=2.*DVDR*DVDR
    ELSE
        TEMP1=0.
    END IF

    TEMP2=(W(I,J,K+1)-W(I,J,K))/ZDF(K)
    TEMP2=TEMP2+0.5*(V(I,J,K)+V(I,J+1,K))
    TEMP=TEMP2/R(J)
    IF(DABS(TEMP).GE.1.E-10) THEN
        TEMP2=2.*TEMP*TEMP
    ELSE
        TEMP2=0.
    END IF

    DUDZ=(U(I+1,J,K)-U(I,J,K))/XDF(I)
    IF(DABS(DUDZ).GE.1.E-10) THEN
        TEMP3=2.*DUDZ*DUDZ
    ELSE
        TEMP3=0.
    END IF
ELSE
  TEMP3=0.
END IF

C
  TEMP=WJAVG(I,J+1,K)+WJAVG(I,J+1,K+1)
  TEMP=TEMP-(WJAVG(I,J,K)+WJAVG(I,J,K+1))
  DWDR(I,J,K)=0.5*TEMP/YDF(J)
  WR(I,J,K)=0.5*(W(I,J,K)+W(I,J,K+1))/R(J)
  TEMP=VKAVG(I,J,K+1)+VKAVG(I,J+1,K+1)
  TEMP=TEMP-(VKAVG(I,J,K)+VKAVG(I,J,K+1))
  DVD=0.5*TEMP/(R(J)*ZDF(K))
  TEMP=DWDR(I,J,K)-WR(I,J,K)+DVDO
  IF(DABS(TEMP).GE.1.E-10) THEN
    TEMP4=TEMP*TEMP
  ELSE
    TEMP4=0.
  END IF
C
  TEMP=WIAVG(I+1,J,K)+WIAVG(I+1,J,K+1)
  TEMP=TEMP-(WIAVG(I,J,K)+WIAVG(I,J,K+1))
  DWDZ=0.5*TEMP/XDF(I)
  TEMP=UKAVG(I+1,J,K+1)+UKAVG(I,J,K+1)
  TEMP=TEMP-(UKAVG(I+1,J,K)+UKAVG(I,J,K))
  DUD=0.5*TEMP/(R(J)*ZDF(K))
  TEMP=DWDZ+DUD
  IF(DABS(TEMP).GE.1.E-10) THEN
    TEMP5=TEMP*TEMP
  ELSE
    TEMP5=0.
  END IF
C
  TEMP=UJAVG(I+1,J+1,K)+UJAVG(I+1,J,K)
  TEMP=TEMP-(UJAVG(I+1,J,K)+UJAVG(I,J,K))
  DUDR=0.5*TEMP/YDF(J)
  TEMP=VIAVG(I+1,J+1,K)+VIAVG(I+1,J,K)
  TEMP=TEMP-(VIAVG(I,J+1,K)+VIAVG(I,J,K))
  DVDZ=0.5*TEMP/XDF(I)
  TEMP=DUDR+DVDZ
  IF(DABS(TEMP).GE.1.E-10) THEN
    TEMP6=TEMP*TEMP
  ELSE
    TEMP6=0.
  END IF
C
  G1(I,J,K)=TEMP1+TEMP2+TEMP3+TEMP4+TEMP5+TEMP6
C
  IF(ZK(I,J,K).GE.1.D-10) THEN
    CON(I,J,K)=ZMUT(I,J,K)*G1(I,J,K)
    CP(I,J,K)=-(RHO(I,J,K)*ZK2(I,J,K))/ZK(I,J,K)
  ELSE
    CP(I,J,K)=0.
  END IF
C
  CP(I,J,K)=CP(I,J,K)-1./DTLAX(NVAR)
CON(I,J,K) = CON(I,J,K) + VAR(I,J,K,NVAR)/DTLAX(NVAR)

IF(ITER.LT.1) GO TO 2600

TEMP = 100. * DABS(CP(I,J,K)) - DABS(CON(I,J,K))

IF(TEMP.LE.0.) CALL CONCP(CON(I,J,K), CP(I,J,K), VAR(I,J,K,NVAR))

2600 CONTINUE
RETURN

ENTRY SORK2

SOURCE TERM FOR E

IF(ITER.EQ.0) THEN
CE = 0.2
END IF

DO 2700 K = KST, KPT1
DO 2700 J = JST, JPT1
DO 2700 I = IST, IPT1

TEMP1 = 0.
IF(CMU(I,J,K).LT.1.D-10) GO TO 2710
IF(ZK(I,J,K).LT.1.D-10) GO TO 2710

F1 = 1.
IF(DABS(CMU(I,J,K)).LT.5.) F1 = 1. + (0.0045/CMU(I,J,K))**3
C1 = 1.44 * F1

TEMP1 = C1 * CMU(I,J,K) * RHO(I,J,K) * ZK(I,J,K) * G1(I,J,K)

2710 CONTINUE

IF(DABS(RT(I,J,K)).LT.1.E-5) THEN
TEMP = 1.
ELSE IF(DABS(RT(I,J,K)).GT.5.) THEN
TEMP = 0.
ELSE
TEMP = DEXP(-RT(I,J,K)**2)
END IF
F2 = 1. - TEMP
C2 = 1.92 * F2

TEMP2 = C2 * RHO(I,J,K) * ZK2(I,J,K)/(ZK(I,J,K)+OVFLW)

CON(I,J,K) = TEMP1 + TEMP2 * ZK2(I,J,K)
CP(I,J,K) = -2. * TEMP2


TEMP = C2 * CC * RHO(I,J,K) * ZK(I,J,K) * WR(I,J,K)

CON(I,J,K) = CON(I,J,K) + TEMP * WR(I,J,K)
TEMP3 = TEMP * DWDR(I,J,K)
IF(TEMP3.GE.0.) THEN
CON(I,J,K) = CON(I,J,K) + TEMP3
ELSE
CP(I,J,K) = CP(I,J,K) + TEMP3/(ZK2(I,J,K)+OVFLW)
END IF

CP(I,J,K) = CP(I,J,K) - 1./DTLAX(NVAR)

CON(I,J,K) = CON(I,J,K) + VAR(I,J,K,NVAR)/DTLAX(NVAR)
IF(ITER.LT.1) GO TO 2700
C
TEMP=100. *DABS(CP(I,J,K)) - DABS(CON(I,J,K))
C
IF(TEMP.LE.0.) CALL CONCP(CON(I,J,K),CP(I,J,K),VAR(I,J,K,NVAR))

2700 CONTINUE
RETURN
END

C
C==============================================================================

SUBROUTINE SOURCN
C==============================================================================

C A SUBROUTINE FOR THE SOURCE TERMS IN NONISOTROPIC MODEL.
C COMPARABLE TO SUBROUTINE SOURCE FOR ISOTROPIC MODEL.
C SOURCE AND SOURCN SHOULD NOT BE IN THIS PROGRAM AT THE SAME TIME.
C
IMPLICIT REAL*8 (A-H,O-Z)
COMMON/VARS/ VAR(30,26,25,14)
COMMON/CALN/ CP(30,26,25),CON(30,26,25), &
CIP(30,26,25),CIM(30,26,25),
&
CJP(30,26,25),CJM(30,26,25),
&
CKP(30,26,25),CKM(30,26,25)
COMMON/VELAVG/ UJAVG(30,26,25),VIAVG(30,26,25),WIAVG(30,26,25), &
UAVG(30,26,25),VAVG(30,26,25),WAVG(30,26,25)
COMMON/PROP/RHOIWT(30,26,25),RHOJWT(30,26,25),RHOKWT(30,26,25), &
GAMIWT(30,26,25),GAMJWT(30,26,25),GAMKWT(30,26,25), &
RHOIED(30,26,25),RHOJED(30,26,25),RHOKED(30,26,25), &
GAMIED(30,26,25),GAMJED(30,26,25),GAMKED(30,26,25)
COMMON/NODES/
&
X(30),XU(30),XDG(30),XDF(30),XDSG(30), &
Y(30),YV(30),YDG(30),YDF(30),YDSG(30), &
Z(30),ZW(30),ZDG(30),ZDF(30),ZDSG(30), &
YDFR(30),YDSGR(30),ARX(30),ARXJ(30),ARXJP(30), &
XDFI(30),XDFIP(30),ZDFK(30),ZDFKP(30), &
R(30),RMN(30),YW(30), &
VOLM(30,26,25),VOLV(30,26,25), &
VOLW(30,26,25)
COMMON/WTING/
&
FX(30),FXM(30),FY(30),FYM(30),FV(30),FVP(30), &
FZ(30),FZM(30)
COMMON/NUMBER/
&
NVAR,MAYVAR,NW,NZMUT,NGAM,NRHO, &
NV,NRW,NU,NPC,NP,NK,NK2
COMMON/ITER1/ ITER,LAST,TIME,DT
COMMON/NPTS/ IPT,IPT1,IPT2,JPT,JPT1,JPT2,KPT,KPT1,KPT2
COMMON/FIRST/ IST,JST,KST
COMMON/GAMLAM/ ZMUL
COMMON/SOR1/ GZ,GC,PATM
COMMON/SORNON/ SRR(30,26,25),SOO(30,26,25),SZZ(30,26,25), &
SOZ(30,26,25),SRO(30,26,25), &
SRRIWT(30,26,25),SRRJWT(30,26,25),SRRKW(30,26,25), &
SOOIWT(30,26,25),SOOJWT(30,26,25),SOOKWT(30,26,25), &
SZZIWT(30,26,25),SZZZWT(30,26,25),SZKWT(30,26,25), &
SOZIWT(30,26,25),SOZZWT(30,26,25),SOZKWT(30,26,25), &
SROIWT(30,26,25),SROJWT(30,26,25),SROKWT(30,26,25),
& SRIED(30,26,25),SRJRED(30,26,25),SRRKED(30,26,25),
& SOOIED(30,26,25),SOOJED(30,26,25),SOOKED(30,26,25),
& SZIED(30,26,25),SZJED(30,26,25),SZKED(30,26,25),
& SOZIED(30,26,25),SOZJED(30,26,25),SOZKED(30,26,25),
& SRJED(30,26,25),SROIED(30,26,25),SROJED(30,26,25),SROKED(30,26,25)
COMMON/OVERFL/ OVFLW
COMMON/SORTUR/ CMU(30,26,25),RT(30,26,25)
COMMON/LAXDT/ DTLAX(14)
DIMENSION G1(30,26,25)
DIMENSION DWR(30,26,25),WR(30,26,25)
DIMENSION U(30,26,25),V(30,26,25),PC(30,26,25),P(30,26,25),
& RW(30,26,25),W(30,26,25),ZK(30,26,25),ZK2(30,26,25),
& ZMUT(30,26,25),GAM(30,26,25),RHO(30,26,25)
EQUIVALENCE
& (VAR(1,1,1,1),V(1,1,1,1)),(VAR(1,1,1,2),RW(1,1,1,1)),
& (VAR(1,1,1,3),U(1,1,1,1)),
& (VAR(1,1,1,4),P(1,1,1,1)),(VAR(1,1,1,5),PC(1,1,1,1)),
& (VAR(1,1,1,6),ZK(1,1,1,1)),(VAR(1,1,1,7),ZK2(1,1,1,1))
EQUIVALENCE
& (VAR(1,1,1,11),W(1,1,1,1)),(VAR(1,1,1,12),ZMUT(1,1,1,1)),
& (VAR(1,1,1,13),GAM(1,1,1,1)),(VAR(1,1,1,14),RHO(1,1,1,1))

C
C =======================================================================

C ENTRY SORV
C
C DO 2100 K=KST,KPT1
DO 2100 J=JST,JPT1
DO 2100 I=IST,IPT1
    TEMP= 0.5* (WJAVG(I,J,K)+WJAVG(I,J,K+1))

    CON(I,J,K)= RHOJWT(I,J,K)*TEMP**2/RMN(J)

    TEMP1=R(J)*GAM(I,J,K)/YDF(J)
    TEMP2=R(J-1)*GAM(I,J-1,K)/YDF(J-1)
    TEMP1=TEMP1**2./SRR(I,J,K)
    TEMP2=TEMP2**2./SRR(I,J-1,K)
    IF(J.EQ.JST) THEN
      TEMP3=R(J)*GAM(I,J,K)/YDF(J-1)
      TEMP2=TEMP2**2./SRR(I,J,K)
    ELSE IF(J.EQ.JPT1) THEN
      TEMP1=R(JPT1)*GAM(I,JPT,K)/YDF(J)
      TEMP1=TEMP1**2./SRR(I,JPT,K)
    END IF
    TEMP3= (TEMP1-TEMP3)*V(I,J+1,K)
    +(TEMP2-TEMP3)*V(I,J-1,K) +(TEMP3+TEMP3)*V(I,J,K)

    TEMP = RMN(J)*YDSG(J)
    CON(I,J,K)=CON(I,J,K)+TEMP3/TEMP
    CP(I,J,K)= -(TEMP1+TEMP2)/TEMP

    IF(J.EQ.JST) THEN
      TEMP41=(W(I,J,K+1)-W(I,1,K+1))/YDSG(J)
      TEMP42=(W(I,J,K)-W(I,1,K))/YDSG(J)
    ELSE IF(J.EQ.JPT1) THEN
      TEMP41=(W(I,JPT,K+1)-W(I,J-1,K+1))/YDSG(J)
      TEMP42=(W(I,JPT,K)-W(I,J-1,K))/YDSG(J)
ELSE
    TEMP41 = (W(I,J,K+1)-W(I,J-1,K+1))/YDSG(J)
    TEMP42 = (W(I,J,K)-W(I,J-1,K))/YDSG(J)
END IF
    TEMP41 = (GAMIED(I,J,K+1)/SROIED(I,J,K+1))
    & (TEMP41-WJAVG(I,J,K+1)/RMN(J))
    TEMP42 = (GAMIED(I,J,K)/SROIED(I,J,K))
    & (TEMP42-WJAVG(I,J,K)/RMN(J))
    CON(I,J,K) = CON(I,J,K)+(TEMP41-TEMP42)/(ZDF(K)*RMN(J))
ENDIF
    IF(J.EQ.JST) THEN
        IF(I.EQ.1ST) THEN
            TEMP51 = GAMKED(I,J,K)*(U(I,J,K)-U(I,1,K))/YDSG(J)
            TEMP52 = TEMP51
        ELSE IF(J.EQ.JPT1) THEN
            IF(I.EQ.1ST) THEN
                TEMP51 = GAMKED(I,J,K)*(U(I,JPT,K)-U(I,J-1,K))/YDSG(J)
                TEMP52 = TEMP51
            ELSE
                IF(I.EQ.1ST) THEN
                    TEMP51 = GAMKED(I,J,K)*(U(I,J,K)-U(I,J-1,K))/YDSG(J)
                    TEMP52 = TEMP51
                ELSE
                    IF(I.EQ.1ST) THEN
                        TEMP51 = GAMKED(I,J,K)*(U(I,J,K)-U(I,J-1,K))/YDSG(J)
                        TEMP52 = TEMP51
                    ELSE
                        TEMP51 = GAMKED(I,J,K)*(U(I,J,K)-U(I,J-1,K))/YDSG(J)
                        TEMP52 = TEMP51
                    END IF
                    CON(I,J,K) = CON(I,J,K)+(TEMP51-TEMP52)/(XDF(I))
    ELSE
        IF(SOOJWT(I,J,K).GT.O.) THEN
            CP(I,J,K) = CP(I,J,K)-TEMP67
        ELSE
            CON(I,J,K) = CON(I,J,K)-TEMP67*V(I,J,K)
        END IF
        TEMP67 = GAMJWT(I,J,K)/SOOJWT(I,J,K)
        TEMP67 = 2.*TEMP67/RMN(J)**2
        TEMP6 = (WJAVG(I,J,K+1)-WJAVG(I,J,K))/ZDF(K)
        CON(I,J,K) = CON(I,J,K)-TEMP67*TEMP6
    IF(SOOJWT(I,J,K).GT.O.) THEN
        CP(I,J,K) = CP(I,J,K)-TEMP67
    ELSE
        CON(I,J,K) = CON(I,J,K)-TEMP67*V(I,J,K)
    END IF
    TEMP81 = GAMIED(I,J,K+1)/ZDG(K+1)
    TEMP82 = GAMIED(I,J,K)/ZDG(K)
    TEMP1 = TEMP81/SROIED(I,J,K+1)
    TEMP2 = TEMP82/SROIED(I,J,K)
    TEMP8 = (TEMP1-TEMP81)*V(I,J,K+1)
    & (TEMP2-TEMP82)*V(I,J,K-1) +(TEMP81+TEMP82)*V(I,J,K)
    TEMP = ZDF(K)*RMN(J)**2
    CON(I,J,K) = CON(I,J,K)+TEMP8/TEMP
    CP(I,J,K) = CP(I,J,K)-(TEMP1+TEMP2)/TEMP
    IF(ITER.LT.1) GO TO 2100
    TEMP = 100.*DBLS(CP(I,J,K)) - DBLS(CON(I,J,K))
    IF(TMP.LE.0.) CALL CONCP(CON(I,J,K),CP(I,J,K),VAR(I,J,K,NVAR))
2100 CONTINUE
RETURN

ENTRY SORW

DO 2200 K=KST,KPT1
DO 2200 J=JST,JPT1
DO 2200 I=IST,IPT1

TEMP2 = 2./YDFR(J)
TEMP21= (GAMIED(I,J+1,K)/SROIED(I,J+1,K))*RMN(J+1)
TEMP22= (GAMIED(I,J,K)/SROIED(I,J,K)) *RMN(J)*WJAVG(I,J,K)

IF(J.EQ.2 OR J.EQ.JPT1) THEN
CP(I,J,K)= 0.
Temp= TEMP21*WJAVG(I,J+1,K) - TEMP22
CON(I,J,K)= -TEMP2*TEMP
ELSE
TEMP= TEMP21/YDSGR(J+1)
CP(I,J,K)= -TEMP2*TEMP *ARXJP(J)
Temp= TEMP*ARXJ(J+1)*W(I,J+1,K) - TEMP22
CON(I,J,K)= -TEMP2*TEMP
END IF

IF(K.EQ.KST) THEN
TEMP31=(V(I,J+1,K)-V(I,J+1,1))/ZDSG(K)
TEMP32=(V(I,J,K)-V(I,J,1))/ZDSG(K)
ELSE IF(K.EQ.KPT1) THEN
TEMP31=(V(I,J+1,KPT)-V(I,J+1,K-1))/ZDSG(K)
TEMP32=(V(I,J,KPT)-V(I,J,K-1))/ZDSG(K)
ELSE
TEMP31=(V(I,J+1,K)-V(I,J+1,K-1))/ZDSG(K)
TEMP32=(V(I,J,K)-V(I,J,K-1))/ZDSG(K)
END IF
TEMP31=TEMP31 *RMN(J+1)*GAMIED(I,J+1,K)/SROIED(I,J,K)
TEMP32=TEMP32 *RMN(J)*GAMIED(I,J,K)/SROIED(I,J,K)
CON(I,J,K)=CON(I,J,K)+(TEMP31-TEMP32)/YDFR(J)

TEMP41=GAM(I,J,K)/ZDF(K)
TEMP42=GAM(I,J,K-1)/ZDF(K-1)
TEMP1=TEMP41*2./SOO(I,J,K)
TEMP2=TEMP42*2./SOO(I,J,K-1)
IF(K.EQ.KST) THEN
TEMP42=GAM(I,J,1)/ZDF(K)
TEMP1=TEMP42*2./SOO(I,J,1)
ELSE IF(K.EQ.KPT1) THEN
TEMP41=GAM(I,J,KPT)/ZDF(K)
TEMP1=TEMP41*2./SOO(I,J,KPT)
END IF
TEMP4= (TEMP1-TEMP41)*RW(I,J,K+1)
& +(TEMP2-TEMP42)*RW(I,J,K-1) +(TEMP41+TEMP42)*RW(I,J,K)
TEMP=R(J)**2 *ZDSG(K)
CON(I,J,K)=CON(I,J,K)+TEMP4/TEMP
CP(I,J,K)=CP(I,J,K)-(TEMP1+TEMP2)/TEMP

TEMP51=0.5*GAM(I,J,K)*(V(I,J+1,K)+V(I,J,K))/SOO(I,J,K)
\[ \text{TMP52} = 0.5 \cdot \text{GAM}(I,J,K-1) \cdot (V(I,J+1,K-1)+V(I,J,K-1))/\text{SOO}(I,J,K-1) \]

IF\((K \text{ EQ. KST})\) THEN
\[ \text{TMP52} = 0.5 \cdot \text{GAM}(I,J,1) \cdot (V(I,J+1,1)+V(I,J,1))/\text{SOO}(I,J,1) \]
ELSE IF\((K \text{ EQ. KPT})\) THEN
\[ \text{TMP52} = 0.5 \cdot \text{GAM}(I,J,KPT) \cdot (V(I,J+1,KPT)+V(I,J,KPT))/\text{SOO}(I,J,KPT) \]
END IF
\[ \text{CON}(I,J,K) = \text{CON}(I,J,K) + 2 \cdot (\text{TMP51} - \text{TMP52})/(R(J) \cdot \text{ZDSG}(K)) \]

C

IF\((K \text{ EQ. KST})\) THEN
IF\((I \text{ EQ. IST})\) THEN
\[ \text{TMP61} = (U(I,J,K)-U(I,J,1))/\text{ZDSG}(K) \]
\[ \text{TMP62} = \text{TMP61} \]
\[ \text{TMP61} = (U(I+1,J,K)-U(I+1,J,1))/\text{ZDSG}(K) \]
ELSE IF\((K \text{ EQ. KPT})\) THEN
\[ \text{TMP61} = (U(I,J,KPT)-U(I,J,K-1))/\text{ZDSG}(K) \]
\[ \text{TMP62} = \text{TMP61} \]
\[ \text{TMP61} = (U(I+1,J,KPT)-U(I+1,J,K-1))/\text{ZDSG}(K) \]
ELSE
\[ \text{TMP61} = (U(I,J,K)-U(I,J,K-1))/\text{ZDSG}(K) \]
\[ \text{TMP62} = \text{TMP61} \]
\[ \text{TMP61} = (U(I+1,J,K)-U(I+1,J,K-1))/\text{ZDSG}(K) \]
ENDIF
\[ \text{TMP61} = \text{TMP61} \cdot \text{GAM JED}(I+1,J,K)/\text{SOZJED}(I+1,J,K) \]
\[ \text{TMP62} = \text{TMP62} \cdot \text{GAM JED}(I,J,K)/\text{SOZJED}(I,J,K) \]
\[ \text{CON}(I,J,K) = \text{CON}(I,J,K) + (\text{TMP61} - \text{TMP62})/\text{XDF}(I) \]
C
\[ \text{TMP71} = \text{RMN}(J+1) \cdot \text{GAM JED}(I,J+1,K)/\text{YDG}(J+1) \]
\[ \text{TMP72} = \text{RMN}(J) \cdot \text{GAM JED}(I,J,K)/\text{YDG}(J) \]
\[ \text{TMP1} = \text{TMP71} / \text{SOZ JED}(I,J+1,K) \]
\[ \text{TMP2} = \text{TMP72} / \text{SOZ JED}(I,J,K) \]
\[ \text{ TEMP} = (\text{TMP1} - \text{TMP71}) \cdot \text{RW}(I,J+1,K) + (\text{TMP1} + \text{TMP72}) \cdot \text{RW}(I,J,K) \]
\[ \text{CON}(I,J,K) = \text{CON}(I,J,K) + \text{TMP7}/\text{YDFR}(J) \]
C
\[ \text{CP}(I,J,K) = \text{CP}(I,J,K) - (\text{TMP1} + \text{TMP2})/\text{YDFR}(J) \]
C
\[ \text{TEMP81} = \text{GAM JED}(I+1,J,K)/\text{XDG}(I+1) \]
\[ \text{TEMP82} = \text{GAM JED}(I,J,K)/\text{XDG}(I) \]
\[ \text{TMP1} = \text{TEMP81} / \text{SOZIED}(I+1,J,K) \]
\[ \text{TMP2} = \text{TEMP82} / \text{SOZIED}(I,J,K) \]
\[ \text{TEMP} = (\text{TMP1} - \text{TEMP81}) \cdot \text{RW}(I+1,J,K) + (\text{TMP1} + \text{TEMP82}) \cdot \text{RW}(I,J,K) \]
\[ \text{CON}(I,J,K) = \text{CON}(I,J,K) + \text{TEMP8}/\text{XDF}(I) \]
C
\[ \text{IF(TEMP.GT.0.) THEN} \]
\[ \text{CP}(I,J,K) = \text{CP}(I,J,K) - \text{TEMP}/\text{XDF}(I) \]
ELSE
\[ \text{CON}(I,J,K) = \text{CON}(I,J,K) - \text{RW}(I,J,K)*\text{TEMP}/\text{XDF}(I) \]
END IF
C
\[ \text{CP}(I,J,K) = \text{CP}(I,J,K) - 1./\text{DTLAX}(\text{NVAR}) \]
C
\[ \text{CON}(I,J,K) = \text{CON}(I,J,K) + \text{VAR}(I,J,K,\text{NVAR})/\text{DTLAX}(\text{NVAR}) \]
C
C
\[ \text{IF(ITER.LT.1) GO TO 2200} \]
C
\[ \text{TEMP} = 100. \cdot \text{DABS}(\text{CP}(I,J,K)) - \text{DABS}(\text{CON}(I,J,K)) \]
C
\[ \text{IF(TEMP.LE.0.) CALL CONCP}(\text{CON}(I,J,K),\text{CP}(I,J,K),\text{VAR}(I,J,K,\text{NVAR})) \]
2200 \text{CONTINUE}
RETURN

C

ENTRY SORU

C

DO 2300 K=KST,KPT1
DO 2300 J=JST,JPT1
DO 2300 I=IST,IPT1
  CON(I,J,K)= RHO1WT(I,J,K)*GZ/GC

C

IF(I.EQ.IST) THEN
  TEMP31=(V(I,J+1,K)-V(1,J+1,K))/XDSG(I)
  TEMP32=(V(I,J,K)-V(1,J,K))/XDSG(I)
ELSE IF(I.EQ.IPT1) THEN
  TEMP31=(V(IPT,J+1,K)-V(I-1,J+1,K))/XDSG(I)
  TEMP32=(V(IPT,J,K)-V(I-1,J,K))/XDSG(I)
ELSE
  TEMP31=(V(I,J+1,K)-V(I-1,J+1,K))/XDSG(I)
  TEMP32=(V(I,J,K)-V(I-1,J,K))/XDSG(I)
END IF
  TEMP31=RMN(J+1)*GAMKED(I,J+1,K)*TEMP31
  TEMP32=RMN(J)*GAMKED(I,J,K)*TEMP32
  CON(I,J,K)=CON(I,J,K)+(TEMP31-TEMP32)/YDFR(J)

C

IF(I.EQ.IST) THEN
  TEMP41=(W(I,J,K+1)-W(1,J,K+1))/XDSG(I)
  TEMP42=(W(I,J,K)-W(1,J,K))/XDSG(I)
ELSE IF(I.EQ.IPT1) THEN
  TEMP41=(W(IPT,J,K+1)-W(I-1,J,K+1))/XDSG(I)
  TEMP42=(W(IPT,J,K)-W(I-1,J,K))/XDSG(I)
ELSE
  TEMP41=(W(I,J,K+1)-W(I-1,J,K+1))/XDSG(I)
  TEMP42=(W(I,J,K)-W(I-1,J,K))/XDSG(I)
END IF
  TEMP41=TEMP41*GAMJED(I,J,K+1)*TEMP41/S0ZJED(I,J,K+1)
  TEMP42=TEMP41*GAMJED(I,J,K)/S0ZJED(I,J,K)
  CON(I,J,K)=CON(I,J,K)+(TEMP41-TEMP42)/(R(J)*ZDF(K))

C

TEMP51=GAM(I,J,K)/XDF(I)
  TEMP52=GAM(I-1,J,K)/XDF(I-1)
  TEMP1=TEMP51*2./SZZ(I,J,K)
  TEMP2=TEMP52*2./SZZ(I-1,J,K)
IF(I.EQ.IST) THEN
  TEMP52=GAM(1,J,K)/XDF(I-1)
  TEMP2=TEMP52*2./SZZ(I,J,K)
ELSE IF(I.EQ.IPT1) THEN
  TEMP51=GAM(IPT,J,K)/XDF(I)
  TEMP1=TEMP51*2./SZZ(IPT,J,K)
END IF
  TEMP5=(TEMP1-TEMP51)*U(I+1,J,K)
  &  +(TEMP2-TEMP52)*U(I-1,J,K)
  &  +(TEMP51+TEMP52)*U(I,J,K)
  CON(I,J,K)=CON(I,J,K)+TEMP5/XDSG(I)
CP(I,J,K) = -(TEMP1+TEMP2)/XDSG(I)

TEMP61 = GAMJED(I,J,K+1)/ZDG(K+1)
TEMP62 = GAMJED(I,J,K)/ZDG(K)
TEMP1 = TEMP61/SOZJED(I,J,K+1)
TEMP2 = TEMP62/SOZJED(I,J,K)
TEMP6 = (TEMP1-TEMP61)*U(I,J,K+1)
& *(TEMP2-TEMP62)*U(I,J,K-1)
& +(TEMP61+TEMP62)*U(I,J,K)
TEMP = R(J)**2*ZDF(K)
CON(I,J,K) = CON(I,J,K)+TEMP6/TEMP
TEMP12 = TEMPL+TEMP2
IF(TEMP12.GT.0.) THEN
CP(I,J,K) = CP(I,J,K)-TEMP12/TEMP
ELSE
CON(I,J,K) = CON(I,J,K)-U(I,J,K)*TEMP12/TEMP
END IF

CP(I,J,K) = CP(I,J,K) - 1./DTLAX(NVAR)
CON(I,J,K) = CON(I,J,K) + VAR(I,J,K,NVAR)/DTLAX(NVAR)

IF(ITER.LT.1) GO TO 2300
TEMP = 100.*DABS(CP(I,J,K)) - DABS(CON(I,J,K))
IF(TEMP.LE.0.) CALL CONCP(CON(I,J,K),CP(I,J,K),VAR(I,J,K,NVAR))
2300 CONTINUE
RETURN

C ------- Entry SORK -------
C CALL AVGWJ
CALL AVGUJ
CALL AVGK
CALL AVGUK
CALL AVGV1
CALL AVGW1
C-- Note: AVGI,J,K should be called again here, because V,W,U have
C been corrected after PC eqn was solved.
C
DO 2600 K=KST,KPT1
DO 2600 J=JST,JPT1
DO 2600 I=IST,IPT1
DVDR = (V(I,J+1,K)-V(I,J,K))/YDF(J)
IF(DABS(DVDR).GE.1.E-10) THEN
TEMP1 = 2.*DVDR*DVDR
ELSE
TEMP1 = 0.
END IF

TEMP2 = (W(I,J,K+1)-W(I,J,K))/ZDF(K)
TEMP2 = TEMP2+ 0.5*(V(I,J,K)+V(I,J+1,K))
TEMP = TEMP2/R(J)
IF(DABS(TEMP).GE.1.E-10) THEN
TEMP2 = 2.*TEMP*TEMP
ELSE
  TEMP2=0.
END IF

C
  DUDZ=(U(I+1,J,K)-U(I,J,K))/XDF(I)
  IF(DABS(DUDZ).GE.1.E-10) THEN
    TEMP3=2.*DUDZ*DUDZ
  ELSE
    TEMP3=0.
  END IF
C
  TEMP=WJAVG(I,J+1,K)+WJAVG(I,J+1,K+1)
  TEMP=TEMP -(WJAVG(I,J,K)+WJAVG(I,J,K+1))
  DWDR(I,J,K)= 0.5*TEMP/YDF(J)
  WR(I,J,K)= 0.5*(W(I,J,K)+W(I,J,K+1))/R(J)
  TEMP=UKAVG(I,J,K+1)+UKAVG(I,J+1,K)
  TEMP=TEMP -(UKAVG(I,J,K)+UKAVG(I,J,K+1))
  DVDO=0.5*TEMP/(R(J)*ZDF(K))
  TEMP=DWDR(I,J,K)-WR(I,J,K)+DVDO
  IF(DABS(TEMP).GE.1.E-10) THEN
    TEMP4=TEMP*TEMP
  ELSE
    TEMP4=0.
  END IF
C
  TEMP=WIAVG(I,J+1,K)+WIAVG(I,J+1,K+1)
  TEMP=TEMP -(WIAVG(I,J,K)+WIAVG(I,J,K+1))
  DWDZ=0.5*TEMP/XDF(I)
  TEMP=UKAVG(I+1,J,K+1)+UKAVG(I,J,K)
  TEMP=TEMP -(UKAVG(I+1,J,K)+UKAVG(I,J,K))
  DVDO=0.5*TEMP/(R(J)*ZDF(K))
  TEMP=DWDZ+DVDO
  IF(DABS(TEMP).GE.1.E-10) THEN
    TEMP5=TEMP*TEMP
  ELSE
    TEMP5=0.
  END IF
C
  TEMP=UJAVG(I+1,J,K)+UJAVG(I+1,J,K+1)
  TEMP=TEMP -(UJAVG(I+1,J,K)+UJAVG(I+1,J,K))
  DUDR=0.5*TEMP/YDF(J)
  TEMP=VIAVG(I+1,J+1,K)+VIAVG(I+1,J,K)
  TEMP=TEMP -(VIAVG(I+1,J+1,K)+VIAVG(I+1,J,K))
  DWDVZ=0.5*TEMP/XDF(I)
  TEMP=DUDR+DWDZ
  IF(DABS(TEMP).GE.1.E-10) THEN
    TEMP6=TEMP*TEMP
  ELSE
    TEMP6=0.
  END IF
C
  G1(I,J,K)= TEMP1/SRR(I,J,K) +TEMP2/SSO(I,J,K)
  & +TEMP3/SSZ(I,J,K) +TEMP4/SRO(I,J,K)
  & +TEMP5/SOZ(I,J,K) +TEMP6
C CKK  CON(I,J,K)=ZMUT(I,J,K)*G1(I,J,K)
C CKK  CP(I,J,K)=-(RHO(I,J,K)*ZK2(I,J,K))/(ZK(I,J,K)+OVFLW)
IF(ZK(I,J,K).GE.1.D-10) THEN
  CON(I,J,K)=ZMUT(I,J,K)*G1(I,J,K)
  CP(I,J,K)=-(RHO(I,J,K)*ZK2(I,J,K))/ZK(I,J,K)
ELSE
  CON(I,J,K)=ZMUT(I,J,K)*G1(I,J,K) - RHO(I,J,K)*ZK2(I,J,K)
  CP(I,J,K)= 0.
END IF
C
  TEMP11=GAMKWT(I,J,K+1)/ZDG(K+1)
  TEMP12=GAMKWT(I,J,K)/ZDG(K)
  TEMP1=TEMP11/SOZKWT(I,J,K+1)
  TEMP2=TEMP12/SOZKWT(I,J,K)
  TEMP13= TEMP1*ZK(I,J,K+1) +TEMP2*ZK(I,J,K-1)
  &
  TEMP14= ( TEMP11*ZK(I,J,K+1) +TEMP12*ZK(I,J,K-1) )
  &
  ( ZK(I,J,K)+OVFLW )
  TEMP=R(J)**2*ZDF(K)
  CON(I,J,K)= CON(I,J,K) +TEMP13/TEMP
  CP(I,J,K)= CP(I,J,K) -TEMP14/TEMP
  TEMP12 = TEMP1+TEMP2
IF(TEMP12.GT.0.) THEN
  CP(I,J,K)=CP(I,J,K)-TEMP12/TEMP
ELSE
  CON(I,J,K)=CON(I,J,K)- ZK(I,J,K)* TEMP12/TEMP
END IF
C
  TEMP21=GAMIWT(I+1,J,K)/XDG(I+1)
  TEMP22=GAMIWT(I,J,K)/XDG(I)
  TEMP1=TEMP21/SZZIWT(I+1,J,K)
  TEMP2=TEMP22/SZZIWT(I,J,K)
  TEMP23= TEMP1*ZK(I+1,J,K) +TEMP2*ZK(I-1,J,K)
  &
  TEMP24= (TEMP21*ZK(I+1,J,K) +TEMP22*ZK(I-1,J,K))
  &
  (ZK(I,J,K)+OVFLW )
  TEMP24 = TEMP24 +TEMP1 +TEMP2
  CON(I,J,K)= CON(I,J,K) +TEMP23/XDF(I)
  CP(I,J,K)= CP(I,J,K) -TEMP24/XDF(I)
C
  CP(I,J,K)=CP(I,J,K) - 1./DTLAX(NVAR)
  CON(I,J,K)=CON(I,J,K) + VAR(I,J,K,NVAR)/DTLAX(NVAR)
C
  IF(ITER.LT.1) GO TO 2600
  TEMP=100. *DABS(CP(I,J,K)) - DABS(CON(I,J,K))
  IF(TEMP.LE.0.) CALL CONCP(CON(I,J,K),CP(I,J,K),VAR(I,J,K,NVAR))
2600 CONTINUE
RETURN
C
C ================================================================================
ENTRY SORK2
C ================================================================================
C
  IF(ITER.EQ.0) THEN
  CC=0.2
END IF
DO 2700 K=KST,KPT1
DO 2700 J=JST,JPT1
DO 2700 I=IST,IPT1
TEMP=0.
IF(CMU(I,J,K).LT.1.D-10) GO TO 2710
IF(ZK(I,J,K).LT.1.D-10) GO TO 2710
F1=1.
IF(DABS(CMU(I,J,K)).LT.5.) F1=1.+((0.0045/CMU(I,J,K))**3)
C1=1.44*F1
2710 CONTINUE

C IF(DABS(RT(I,J,K)).LT.1.E-5) THEN
    TEMP=1.
ELSE IF(DABS(RT(I,J,K)).GT.5.) THEN
    TEMP=0.
ELSE
    TEMP=DEXP(-RT(I,J,K)**2)
END IF
F2=1.-TEMP
C2=1.92*F2
TEMP2=C2*RHO(I,J,K)*ZK2(I,J,K)/(ZK(I,J,K)+OVFLW)

C CON(I,J,K)=TEMP1+TEMP2*ZK2(I,J,K)
CP(I,J,K)=-2.*TEMP2

    TEMP =C2*CC*RHO(I,J,K)*ZK(I,J,K)*WR(I,J,K)
    CON(I,J,K)=CON(I,J,K)+TEMP*WR(I,J,K)
    TEMP3 = TEMP*DWDR(I,J,K)
    IF(TEMP3.GE.0.) THEN
        CON(I,J,K)=CON(I,J,K)+TEMP3
    ELSE
        CP(I,J,K)=CP(I,J,K)+TEMP3/(ZK2(I,J,K)+OVFLW)
    END IF

C TEMP11=GAMKW(T(I,J,K+1)/ZDG(K+1)
TEMP12=GAMKW(T(I,J,K)/ZDG(K)
TEMP1=TEMP11/SOZKWT(I,J,K+1)
TEMP2=TEMP12/SOZKWT(I,J,K)
TEMP13= TEMP1*ZK2(I,J,K+1)+TEMP2*ZK2(I,J,K-1)
&
TEMP14= ( TEMP11*ZK2(I,J,K+1) +TEMP12*ZK2(I,J,K-1) )
&
/* ZK2(I,J,K)+OVFLW */
TEMP=R(J)**2*ZDF(K)
CON(I,J,K)= CON(I,J,K) +TEMP13/TEMP
CP(I,J,K)= CP(I,J,K) -TEMP14/TEMP
TEMP12 = TEMP1+TEMP2
IF(TEMP12.GT.0.) THEN
    CP(I,J,K)=CP(I,J,K)-TEMP12/TEMP
ELSE
    CON(I,J,K)=CON(I,J,K)- ZK2(I,J,K)* TEMP12/TEMP
END IF
TEMP21 = GAMIWT(I+1,J,K)/XD(I+1)
TEMP22 = GAMIWT(I,J,K)/XD(I)
TEMP1 = TEMP21/SZIW(T+1,J,K)
TEMP2 = TEMP22/SZIW(T,J,K)
TEMP23 = TEMP1*ZK2(I+1,J,K) + TEMP2*ZK2(I-1,J,K)
& + (TEMP21+TEMP22)*ZK2(I,J,K)
TEMP24 = (TEMP21*ZK2(I+1,J,K) + TEMP22*ZK2(I-1,J,K))
& / (ZK2(I,J,K)+OVFLW)
TEMP24 = TEMP24 + TEMP1 + TEMP2
CON(I,J,K) = CON(I,J,K) + TEMP23/XDF(I)
CP(I,J,K) = CP(I,J,K) - TEMP24/XDF(I)
CP(I,J,K) = CP(I,J,K) - 1./DTLAX(NVAR)
CON(I,J,K) = CON(I,J,K) + VAR(I,J,K,NVAR)/DTLAX(NVAR)
IF(ITER.LT.1) GO TO 2700
TEMP = 100. *DABS(CP(I,J,K)) - DABS(CON(I,J,K))
IF(TEMP.LE.0.) CALL CONCP(CON(I,J,K),CP(I,J,K),VAR(I,J,K,NVAR))
2700 CONTINUE
RETURN
END

SUBROUTINE T3E3D

OTHER ASSISTANT SUBROUTINES FOR THE 3D SIMULATION OF TANK SYSTEM 3

IMPLICIT REAL*8 (A-H,O-Z)
LOGICAL PRESDU,CONVGN
COMMON/QUIT/CONVGN
COMMON/SUMAX/CONTOT,CONMX,RESMAX(14)
COMMON/PRTRIES/PRESDU
COMMON/VARS/ VAR(30,26,25,14)
COMMON/CALN/ CP(30,26,25),CON(30,26,25),
& CIP(30,26,25),CIM(30,26,25),
& CJP(30,26,25),CJM(30,26,25),
& CKP(30,26,25),CKM(30,26,25)
COMMON/PROP/RHOIWT(30,26,25),RHOJWT(30,26,25),RHOKWT(30,26,25),
& GAMIWT(30,26,25),GAMJWT(30,26,25),GAMKWT(30,26,25),
& RHOIED(30,26,25),RHOJED(30,26,25),RHOKED(30,26,25),
& GAMIED(30,26,25),GAMJED(30,26,25),GAMKED(30,26,25)
COMMON/VELAVG/ UJAVG(30,26,25),VIAVG(30,26,25),WIAVG(30,26,25),
& UKAVG(30,26,25),VKAVG(30,26,25),WJAVG(30,26,25)
COMMON/NODES/
& X(30),XU(30),XD(30),XDF(30),XDSG(30),
& Y(30),YV(30),YDG(30),YDF(30),YDSG(30),
& Z(30),ZW(30),ZDG(30),ZDF(30),ZDSG(30),
& YDFR(30),YDSGR(30),ARX(30),ARXJ(30),ARXJP(30),
& XDFI(30),XDFIP(30),ZDFK(30),ZDFKP(30),
& R(30),RMN(30),YW(30),
& VOLM(30,26,25),VOLV(30,26,25),
& VOLW(30,26,25),VOLUM(30,26,25)
COMMON/WTING/
& FX(30),FXM(30),FY(30),FYM(30),FV(30),FVP(30),
& FZ(30),FZM(30)
COMMON/SHAPE/ XL,YL,ZL
COMMON/PELLER/ DIMPEL,RPM
COMMON/BAFFLE/ JBAFFL
COMMON/BCPLLR/ VIBC(6),WIBC(6),UBWC(7)
COMMON/NPPTS/ IPT,IP1,IP2,JPT,JPT1,JPT2,KPT,KPT1,KPT2
COMMON/NUMBER/
& NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
& NV,NRW,NU,NPC,NP,NK,NK2
COMMON/ITER/ ITER,LAST,TIME,DT
COMMON/DEN/ RHOCON
COMMON/GAMLAM/ ZMUL
COMMON/SORI/ GZ,GC,PATH
COMMON/SORTUR/ CMU(30,26,25),RT(30,26,25)
COMMON/LAXDT/ DTLAX(14)
COMMON/OVERFL/ OVFLW
COMMON/BIOLUM/ BIG
COMMON/PAI/ PI
DIMENSION U(30,26,25),V(30,26,25),PC(30,26,25),P(30,26,25),
& RW(30,26,25),W(30,26,25),ZK(30,26,25),ZK2(30,26,25),
& ZMUT(30,26,25),GAM(30,26,25),RHO(30,26,25)
DIMENSION UOLD(30,26,25),VOLD(30,26,25),
& RWOLD(30,26,25),ZKOLD(30,26,25),ZK2OLD(30,26,25)
DIMENSION UBLA(30,26,25),VBLA(30,26,25),WBLA(30,26,25),
& RWBLA(30,26,25),ZKB(30,26,25),ZKBLA(30,26,25),ZK2BLA(30,26,25),
& PBLA(30,26,25),PCBLA(30,26,25)
EQUIVALENCE
& (VAR(1,1,1,1),V(1,1,1)),(VAR(1,1,1,2),RW(1,1,1)),
& (VAR(1,1,1,3),U(1,1,1)),
& (VAR(1,1,1,4),P(1,1,1)),(VAR(1,1,1,5),PC(1,1,1)),
& (VAR(1,1,1,6),ZK(1,1,1)),(VAR(1,1,1,7),ZK2(1,1,1))
EQUIVALENCE
& (VAR(1,1,1,11),W(1,1,1)),(VAR(1,1,1,12),ZMUT(1,1,1)),
& (VAR(1,1,1,13),GAM(1,1,1)),(VAR(1,1,1,14),RHO(1,1,1))

C
C ---------------------------------------------
ENTRY VGRID
C
C VARIABLE GRID STRUCTURE
C
C --- Centerline of the tank: XU(16) ------
C XU(16)=0.
C XU(2)=-XL/2.
C --- Tip of impeller blade: YV(9) ------
C YV(9)=DIMPEL/2.
C YV(2)=0.0
C YV(JPT)=YL
C YV(JPT1)=YV(JPT)-1./16.
C --- Degrees are measured from a baffle ------
C ZW(2)=0.0
C ZW(KPT)=ZL
C ZW(3)=1.0
C ZW(4)=2.0
C ZW(5)=4.0
ZW(6)=6.0
ZW(7)=9.0
ZW(8)=12.0
ZW(9)=15.0
ZW(10)=18.0
ZW(11)=22.0
ZW(12)=31.0
ZW(13)=41.0
DO 111 K=14,24
111  ZW(K)=ZL-ZW(27-K)
C  IF(DIMPEL.EQ.3.) THEN
   DO 113 J=3,7
113   YV(J)=YV(J-1)+0.25
    YV(8)=YV(9)-0.05
    YV(10)=YV(9)+0.05
    YV(11)=1.66
    YV(12)=1.84
    YV(13)=2.04
    YV(14)=2.34
    YV(15)=2.66
    YV(16)=2.75
   DO 115 J=17,20
115   YV(J)=YV(J-1)+0.5
    YV(21)=4.94
    YV(22)=5.06
    YV(23)=5.32
    YV(24)=5.56
    XU(3)=-5.51
    XU(4)=-5.40
    XU(5)=-5.10
    XU(6)=-4.875
   DO 117 I=7,12
117   XU(I)=XU(I-1)+0.75
    XU(13)=-0.30
    XU(14)=-0.20
    XU(15)=-0.10
C  ELSE IF(DIMPEL.EQ.4.0) THEN
   XU(3)=-5.51
   XU(4)=-5.40
   XU(5)=-5.10
   XU(6)=-4.875
   DO 133 I=7,11
133   XU(I)=XU(I-1)+0.75
   XU(12)=-0.475
   XU(13)=-0.40
   XU(14)=-0.25
   XU(15)=-0.10
C  IF(RPM.EQ.150.0) THEN
   DO 135 J=3,7
135   YV(J)=YV(J-1)+0.375
    YV(8)=YV(9)-0.05
    YV(10)=2.04
YV(11)=2.20
YV(12)=2.37
YV(13)=2.87
YV(14)=3.37
YV(15)=3.87
YV(16)=4.13
YV(17)=4.87
YV(18)=5.08
YV(19)=5.30
YV(20)=5.40
YV(21)=5.60
ELSE IF(RPM.EQ.200.0) THEN
  DO 155 J=3,7
    YV(J)=YV(J-1)+0.375
  YV(8)=YV(9)-0.05
  YV(10)=2.04
  YV(11)=2.34
  YV(12)=2.66
  YV(13)=2.75
  DO 157 J=14,17
    YV(J)=YV(J-1)+0.5
  YV(18)=4.94
  YV(19)=5.06
  YV(20)=5.32
  YV(21)=5.56
END IF
END IF

DO 181 I=17,IPT
  XU(I)=-XU(IPT+2-I)
  DO 183 I=2,IPT
    XU(I)=XU(I)+XL/2.

DO 190 K=2,KPT
  ZW(K)=ZW(K)*PI/180.0
  DO 191 I=2,IPT
    XU(I)=XU(I)/12.
  DO 193 J=2,JPT
    YV(J)=YV(J)/12.
    DIMPEL=DIMPEL/12.
    XL=XL/12.
    YL=YL/12.
    ZL=ZL*PI/180.
    RETURN

ENTRY GAMFAC(RATIO)
ENTRY EXCHANGE COEFFICIENT RATIOS

IF(NVAR.EQ.NK) THEN
  SIGK=0.87
  RATIO=SIGK
ELSE IF(NVAR.EQ.NK2) THEN
SIGK2=1.3
RATIO=SIGK2
ELSE
RATIO=1.0
END IF
RETURN
C
C==============================================================================================
ENTRY TURB
C==============================================================================================
C TURBULENCE MODEL
C
DO 250 K=1,KPT
DO 250 J=1,JPT
DO 250 I=1,IPT
C --- To avoid divide check ---
IF(ZK(I,J,K).LT.1.D-10) THEN
RT(I,J,K)=0.
CMU(I,J,K)=0.
ELSE
RT(I,J,K)=RHO(I,J,K)*ZK(I,J,K)**2/(ZMUL*ZK2(I,J,K)+OVFLW)
RK=RHO(I,J,K)*ZK(I,J,K)**0.5*YW(J)/ZMUL
TEMP1 = 0.
IF(RK.LT.500.) TEMP1 = DEXP(-0.0165*RK)
TEMP2 = 1.+20.5/RT(I,J,K)
FMU=TEMP2*(1.-TEMP1)**2
CMU(I,J,K)=0.09*FMU
END IF
ZMUT(I,J,K)=CMU(I,J,K)*RHO(I,J,K)*ZK(I,J,K)**2 /
/(ZK2(I,J,K)+OVFLW)
250 CONTINUE
RETURN
C
C==============================================================================================
ENTRY INITIA
C==============================================================================================
C --- Variables are initialized here -----
C
37 FORMAT(1X,I2,1X,1P,6E12.4,2X,I2)
38 FORMAT(1X,I2,1X,1P,6E12.4)
IFST=1
JFST=1
DO 290 NPHI=1,NK2
IF(NPHI.EQ.NPC) GO TO 290
IBEG=IFST-6
280 CONTINUE
IBEG=IBEG+6
IEND=(IBEG-1)+6
IEND=MIND(IEND,IPT)
INUM=IEND-IBEG+1
DO 285 JJ=JFST,JPT
J=JFST+JPT-JJ
IF(INUM.EQ.6) THEN
READ(5,37) JN,(VAR(I,J,1,NPHI),I=IBEG,IEND),JNL
ELSE
READ(5,38) JN,(VAR(I,J,1,NPHI),I=IBEG,IEND)
END IF
285 CONTINUE
IF(IEND.LT.IPT) GO TO 280
290 CONTINUE
CC
C 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9
DO 293 K=2,KPT
DO 293 J=1,JPT
DO 293 I=1,IPT
V(I,J,K)= VAR(I,J,1,NV)
W(I,J,K)= VAR(I,J,1, NRW)
U(I,J,K)= VAR(I,J,1, NU)
P(I,J,K)= VAR(I,J,1, NP)
ZK(I,J,K)= VAR(I,J,1,NK)
ZK2(I,J,K)= VAR(I,J,1,NK2)
293 CONTINUE
CFAC = 0.3048*0.3048
DO 295 K=1,KPT
DO 295 J=1,JPT
DO 295 I=1,IPT
RHO(I,J,K)= RHOCON
V(I,J,K)= V(I,J,K)/0.3048
W(I,J,K)= W(I,J,K)/0.3048
RW(I,J,K)= R(J)*W(I,J,K)
U(I,J,K)= U(I,J,K)/0.3048
P(I,J,K)= P(I,J,K)*2116.2/101330.0
CCC
P(I,J,K)= 0.
CCC
P(I,J,K)= RHOCON*(GZ/GC)*(XL-X(I))
PC(I,J,K) = 0.
ZK(I,J,K) = ZK(I,J,K)/CFAC
ZK2(I,J,K) = ZK2(I,J,K)/CFAC
295 CONTINUE
DO 298 K=1,KPT
DO 298 J=1,J9
DO 298 I=13,19
VBLA(I,J,K)= V(I,J,K)
RWBLA(I,J,K)= RW(I,J,K)
WBLA(I,J,K)= W(I,J,K)
UBLA(I,J,K)= U(I,J,K)
PBLA(I,J,K)= P(I,J,K)
ZKBLA(I,J,K)= ZK(I,J,K)
ZK2BLA(I,J,K)= ZK2(I,J,K)
298 CONTINUE
RETURN
C
C =====================================================================================================
ENTRY BCS
C
C BOUNDARY CONDITIONS
C
DO 300 K=1,KPT
DO 300 I=2,IPT1
   V(I,2,K)=0.
   RW(I,1,K)=0.
   W(I,1,K)=0.
   IF(I.LE.12) THEN
      IF(I.GE.3) U(I,1,K)=U(I,2,K)
      ZK(I,1,K)=ZK(I,2,K)
      ZK2(I,1,K)=ZK2(I,2,K)
   ELSE
      U(I,1,K)=0.
      ZK(I,1,K)=0.
      ZK2(I,1,K)=0.
      P(I,2,K)= RHOCON*(GZ/GC)*(X(I)-X(I))
      PC(I,2,K)=0.
      V(I,3,K)=0.
      RW(I,2,K)=0.
      W(I,2,K)=RW(I,2,K)/R(2)
      IF(ITER.EQ.0) THEN
         TEMP1=YV(3)/R(3)-R(3)/YV(3)
         TEMP2=YV(3)/YL-YL/YV(3)
         WI3 = 2.*PI*(RPM/60.)*YLV/TEMP1/TEMP2
      END IF
      RW(I,3,K)= R(3)*WI3
      W(I,3,K)= WI3
      U(I,2,K)=0.
      ZK(I,2,K)=0.
      ZK2(I,2,K)=0.
   END IF

C
V(I,JPT,K)=.0
RW(I,JPT,K)=.0
   W(I,JPT,K)=RW(I,JPT,K)/R(JPT)
U(I,JPT,K)=.0
ZK(I,JPT,K)=.0
ZK2(I,JPT,K)=.0
C  ZK2(I,JPT,K)=ZK2(I,JPT1,K)
C
C
300 CONTINUE
C
DO 340 K=1,KPT
DO 340 J=1,JPT
   V(1,J,K)=.0
   RW(1,J,K)=.0
   W(1,J,K)=.0
   U(2,J,K)=.0
   ZK(1,J,K)=.0
   ZK2(1,J,K)=.0
C  ZK2(1,J,K)=ZK2(2,J,K)
C
   IF(J.LE.3) V(IPT,J,K)=0.
   IF(J.GE.4) V(IPT,J,K)=V(IPT1,J,K)
   IF(J.LE.2) THEN
      RW(IPT,J,K)=0.
      W(IPT,J,K)=0.
      U(IPT,J,K)=0.
      ZK(IPT,J,K)=0.
ZK2(IPT,J,K)=0.
ELSE
   RW(IPT,J,K)=R(IPT1,J,K)
   W(IPT,J,K)=RW(IPT,J,K)/R(J)
   U(IPT,J,K)=0.
   ZK(IPT,J,K)=ZK(IPT1,J,K)
   ZK2(IPT,J,K)=ZK2(IPT1,J,K)
END IF
CONTINUE
C
DO 360 I=2,IPT1
DO 360 J=2,JPT1
IF(J.NE.2) V(I,J,1)=0.5* (V(I,J,KPT2)+V(I,J,KPT2-1))
RW(I,J,2)=RW(I,J,KPT2)
   W(I,J,2)=RW(I,J,2)/R(J)
IF(J.NE.2) U(I,J,1)=0.5* (U(I,J,KPT2)+U(I,J,KPT2-1))
ZK(I,J,1)=0.5* (ZK(I,J,KPT2)+ZK(I,J,KPT2-1))
ZK2(I,J,1)=0.5* (ZK2(I,J,KPT2)+ZK2(I,J,KPT2-1))
C
IF(J.NE.2) V(I,J,KPT)=0.5* (V(I,J,3)+V(I,J,4))
RW(I,J,KPT)=RW(I,J,4)
   W(I,J,KPT)=RW(I,J,KPT)/R(J)
IF(J.NE.2) U(I,J,KPT)=0.5* (U(I,J,3)+U(I,J,4))
ZK(I,J,KPT)=0.5* (ZK(I,J,3)+ZK(I,J,4))
ZK2(I,J,KPT)=0.5* (ZK2(I,J,3)+ZK2(I,J,4))
IF(J.GE.JBAFFL) THEN
   RW(I,J,3)=.0
   W(I,J,3)=.0
   RW(I,J,KPT1)=.0
   W(I,J,KPT1)=.0
END IF
CONTINUE
C
DO 380 K=2,KPT1
DO 380 J=2,9
   U(19,J,K)=UBLA(19,J,K)
DO 380 I=13,19
   IF(J.NE.2) V(I,J,K)=VBLA(I,J,K)
   IF(K.NE.2) RW(I,J,K)=RWBLA(I,J,K)
   IF(K.NE.2) W(I,J,K)=WBLA(I,J,K)
   U(I,J,K)=UBLA(I,J,K)
   P(I,J,K)= PBLA(I,J,K)
   PC(I,J,K)= 0.
   ZK(I,J,K)=ZKBLA(I,J,K)
   ZK2(I,J,K)=ZK2BLA(I,J,K)
CONTINUE
DO 384 K=1,KPT
DO 384 I=13,19
   IF(I.EQ.19) GO TO 384
   V(I,9,K)=VIBC(II)/60.
   W(I,9,K)=WIBC(II)/60.
   RW(I,9,K)=R(9)*W(I,9,K)
IF(NVAR.EQ.NV) THEN
  DO 519 K=2,KPT1
      DO 510 I=13,IPT1
         CON(I,3,K)=BIG*VAR(I,3,K,NVAR)
         CP(I,3,K)=-BIG
      CONTINUE
  DO 515 J=3,39
  DO 515 I=13,18
     CON(I,J,K)=BIG*VAR(I,J,K,NVAR)
     CP(I,J,K)=-BIG
  CONTINUE
  519 CONTINUE

ELSE IF(NVAR.EQ.NRW) THEN
  DO 520 I=2,IPT1
  DO 520 J=JBAFFL,JPT1
     CON(I,J,3)=BIG*VAR(I,J,3,NVAR)
     CP(I,J,3)=-BIG
     CON(I,J,KPT1)=BIG*VAR(I,J,KPT1,NVAR)
     CP(I,J,KPT1)=-BIG
  CONTINUE
  DO 529 K=3,KPT1
  DO 523 I=13,IPT1
      DO 523 J=2,3
         CON(I,J,K)=BIG*VAR(I,J,K,NVAR)
         CP(I,J,K)=-BIG
      CONTINUE
  DO 525 I=13,18
  DO 525 J=2,9
     CON(I,J,K)=BIG*VAR(I,J,K,NVAR)
     CP(I,J,K)=-BIG
  CONTINUE
  529 CONTINUE

ELSE IF(NVAR.EQ.NU) THEN
  DO 539 K=2,KPT1
      DO 530 I=13,IPT1
         CON(I,2,K)=BIG*VAR(I,2,K,NVAR)
         CP(I,2,K)=-BIG
      CONTINUE
  DO 533 J=2,9
  DO 533 I=13,19
     CON(I,J,K)=BIG*VAR(I,J,K,NVAR)
     CP(I,J,K)=-BIG
  CONTINUE
ELSE IF(NVAR.EQ.NP .OR. NVAR.EQ.NPC) THEN
   DO 549 K=2,KPT1
   C --- Shaft -----
   DO 540 I=13,IPT1
      CJM(I,3,K)=0.
      CJP(I,2,K)=0.
      CIM(I,2,K)=0.
      CIP(I-1,2,K)=0.
   CONTINUE
   C --- Blade -----
   DO 544 J=3,9
   DO 544 I=13,18
      CJM(I,J,K)=0.
      CJP(I,J-1,K)=0.
   CONTINUE
   DO 546 J=2,9
   DO 546 I=13,19
      CIM(I,J,K)=0.
      CIP(I-1,J,K)=0.
   CONTINUE
   549 CONTINUE
   C
   DO 557 K=3,KPT1
   DO 553 I=13,IPT1
   DO 553 J=2,3
      CKM(I,J,K)=0.
      CKP(I,J,K-1)=0.
   CONTINUE
   DO 555 I=13,18
   DO 555 J=2,9
      CKM(I,J,K)=0.
      CKP(I,J,K-1)=0.
   CONTINUE
   557 CONTINUE
   C
   ELSE IF(NVAR.EQ.NK .OR. NVAR.EQ.NK2) THEN
   DO 569 K=2,KPT1
   DO 560 I=13,IPT1
      CON(I,2,K)=BIG*VAR(I,2,K,NVAR)
      CP(1,2,K)=BIG
   CONTINUE
   DO 563 I=13,18
   DO 563 J=2,9
      CON(I,J,K)=BIG*VAR(I,J,K,NVAR)
      CP(I,J,K)=-BIG
   CONTINUE
   569 CONTINUE
   C
CONTINUE
ELSE
END IF
RETURN

ENTRY ITERED

ITERATION

20 FORMAT(/,6X,'Iteration values for the grid point ('
& 'I2,'I2,'I2,'I2,')')
21 FORMAT(/,1X,'ITER',2X,'CONTOT',4X,'V',4X,'W',4X,'
& 'U',4X,'ZK',3X,'ZK2',2X,'PC',/)
31 FORMAT(/,2X,'ITER',2X,'CONTOT',4X,'RESMAX;V',3X,'RESMAX;RW',2X,
& 'RESMAX;U',3X,'RESMAX;K',3X,'RESMAX;K2',/)
41 FORMAT(/,2X,'ITER',5X,
& 'Relative Errors for V, RW, U, ZK, and ZK2/')

CF 12 FORMAT(4X,1P,6E12.3/)
CF 13 FORMAT(4X,1P,5E12.3/)
22 FORMAT(5X,I3,1P,6E11.3)
32 FORMAT(1X,I4,5X,1P,5E11.3)
33 FORMAT(1X,I4,5X,1P,5E11.3)

IF(ITER.EQ.0) THEN
PRESDU=.TRUE.
NOLUCK=0
IX= 9
JY=14
KZ= 5
WRITE(8,20) IX,JY,KZ
WRITE(9,20) IX,JY,KZ
WRITE(8,21)
WRITE(9,21)
WRITE(4,31)
WRITE(3,41)
ELSE
ERRV=ABS(V(IX,JY,KZ)-VOLD(IX,JY,KZ))/DENOMV
ERRW=ABS(RW(IX,JY,KZ)-RWOLD(IX,JY,KZ))/DENOMW
ERRU=ABS(U(IX,JY,KZ)-UOLD(IX,JY,KZ))/DENOMU
ERRK=ABS(ZK(IX,JY,KZ)-ZKOLD(IX,JY,KZ))/DENOMK
ERRK2=ABS(ZK2(IX,JY,KZ)-ZK2OLD(IX,JY,KZ))/DENMK2
END IF

DO 343 L=8,8
343 WRITE(L,22) ITER,CONTOT,V(IX,JY,KZ),W(IX,JY,KZ),U(IX,JY,KZ),
& ZK(IX,JY,KZ),ZK2(IX,JY,KZ)

IF(ITER.EQ.0) GO TO 375

IF(ERRV.LT.1.E-5 .AND.
& ERRW.LT.1.E-5 .AND.
& ERRU.LT.1.E-5 .AND.
& RERRK.LT.1.E-5 .AND.
& RERR2.LT.1.E-5) THEN
C IF(RERRV.LT.1.E-4 .AND.
C & RERRW.LT.1.E-4 .AND.
C & RERRU.LT.1.E-4 .AND.
C & RERRK.LT.1.E-4) THEN
C & RERR2.LT.1.E-4 .AND.
C & RESMAX(NV).LT.1.E-3 .AND.
C & RESMAX(NRW).LT.1.E-3 .AND.
C & RESMAX(NV).LT.1.E-3) THEN
NOLUCK=NOLUCK+1
IF(NOLUCK.EQ.4) CONVGN=.TRUE.
ELSE
NOLUCK=0
END IF
C CRES IF(PRESDU) THEN
C WRITE(4,32) ITER,CONTOT,RESMAX(NV),RESMAX(NRW),
C & RESMAX(NU),RESMAX(NK),RESMAX(NK2)
C WRITE(3,33) ITER,RERRV,RERRW,RERRU,RERRK,RERR2
C ELSE
C END IF
C IF(MOD(ITER,1).EQ.0.OR.NOLUCK.GT.0) THEN
C PRESDU=.TRUE.
C ELSE
C PRESDU=.FALSE.
CRES END IF
C C IF(MOD(ITER,20).EQ.1) THEN
C WRITE(9,*)'--- CONTOT, RESMAX for V, RW, U, K, and K2 are:
C WRITE(9,12) CONTOT,(RESMAX(I),I=NV,NU),(RESMAX(I),I=NK,NK2)
C WRITE(9,*)'--- Relative errors for V, RW, U, K, and K2 are:
C WRITE(9,13) RERRV,RERRW,RERRU,RERRK,RERR2
C END IF
C C IF(ITER.GE.LAST) THEN
C WRITE(9,*)'*** NOTE :''LAST,' is the last iteration ***'
C WRITE(9,*)'--- CONTOT, RESMAX for V, RW, U, K, and K2 are:
C WRITE(9,12) CONTOT,(RESMAX(I),I=NV,NU),(RESMAX(I),I=NK,NK2)
C WRITE(9,*)'--- Relative errors for V, RW, U, K, and K2 are:
C WRITE(9,13) RERRV,RERRW,RERRU,RERRK,RERR2
C WRITE(9,*)'*** Input a larger value of LAST for more iteration:
C CCC WRITE(9,*)' (If no more iteration is needed, enter same LAST)'
CCC READ(9,*) LAST
C IF(ITER.GE.LAST) CONVGN=.TRUE.
C ELSE
C END IF
C CONTINUE
C DO 378 I = 2, IPT1
DO 378 J = 2, JPT1
DO 378 K = 2, KPT1
VOLD(I,J,K)=V(I,J,K)
RWOLD(I,J,K)=RW(I,J,K)
378 CONTINUE
UOLD(I,J,K) = U(I,J,K)
ZKOLD(I,J,K) = ZK(I,J,K)
ZK2OLD(I,J,K) = ZK2(I,J,K)

378 CONTINUE

C
IF (DABS(VOLD(IX,JY,KZ)) .LT. 1.E-3) THEN
   DENOMV = DABS(VOLD(IX,JY,KZ)) + 1.
ELSE
   DENOMV = DABS(VOLD(IX,JY,KZ))
END IF
IF (DABS(RWOLD(IX,JY,KZ)) .LT. 1.E-3) THEN
   DENOMW = DABS(RWOLD(IX,JY,KZ)) + 1.
ELSE
   DENOMW = DABS(RWOLD(IX,JY,KZ))
END IF
IF (DABS(UOLD(IX,JY,KZ)) .LT. 1.E-3) THEN
   DENOMU = DABS(UOLD(IX,JY,KZ)) + 1.
ELSE
   DENOMU = DABS(UOLD(IX,JY,KZ))
END IF
IF (DABS(ZKOLD(IX,JY,KZ)) .LT. 1.E-3) THEN
   DENOMK = DABS(ZKOLD(IX,JY,KZ)) + 1.
ELSE
   DENOMK = DABS(ZKOLD(IX,JY,KZ))
END IF
IF (DABS(ZK2OLD(IX,JY,KZ)) .LT. 1.E-3) THEN
   DENOMK2 = DABS(ZK2OLD(IX,JY,KZ)) + 1.
ELSE
   DENOMK2 = DABS(ZK2OLD(IX,JY,KZ))
END IF
RETURN
END

C
==================================================================
C
================== BLOCK DATA
C
==================================================================

IMPLICIT REAL*8 (A-H,O-Z)
LOGICAL SIMPLE,UNIFOM,SOLVE,PRNT,CONVGN,RHOVAR,NOTURB,ONCE,PBCEXT
COMMON/ALGTHM/ SIMPLE
COMMON/VARS/ VAR(30,26,25,14)
COMMON/GRDTYP/UNIFOM
COMMON/RHOV/RHOVAR
COMMON/GAM2/NOTURB,ONCE
COMMON/SOLN/SOLVE(14)
COMMON/PRT/PRNT(14)
CHARACTER*15 TITLE
COMMON/TITLE1/TITLE(14)
COMMON/LAXVAR/RELAX(14)
COMMON/LAX2/ ITRLAX(9),NCHNGE(14)
COMMON/LAX3/ DBETA(9,14)
COMMON/LAXSOR/RELSOR(14)
COMMON/LAXDT/ DTLAX(14)
COMMON/SUMAX/CONTOT,CONTMX,RESMAX(14)
COMMON/QUIT/CONVGN
COMMON/NUMBER/
& NVAR,MAXVAR,NW,NZMUT,NGAM,NRHO,
& NV,NRW,NP,NPC,NP,NK,NK2
COMMON/SOLVST/NSOLST
COMMON/ITER1/ITER,LAST,TIME,DT
COMMON/SHAPE/XL,YL,ZL
COMMON/PELLER/DIMPEL,RPM
COMMON/BAFFLE/JDAFFL
COMMON/BCPLLR/VIBC(6),WIBC(6),UIBC(7)
COMMON/NPTS/IPT,IPT1,IPT2,JPT,JPT1,JPT2,KPT,KPT1,KPT2
COMMON/NODES/
& X(30),XU(30),XDG(30),XDF(30),XDSG(30),
& Y(30),YV(30),YDG(30),YDF(30),YDSG(30),
& Z(30),ZW(30),ZDG(30),ZDF(30),ZDSG(30),
& YDFR(30),YDSGR(30),ARX(30),ARXJ(30),ARXJP(30),
& XDFI(30),XDFIP(30),ZDFK(30),ZDFKP(30),
& R(30),RMN(30),YW(30),
& VOLM(30,26,25),VOLV(30,26,25),
& VOLW(30,26,25),VOLUM(30,26,25)
COMMON/GAMLAM/ ZMJL
COMMON/DEN/ RHOCON
COMMON/SOR1/ GZ,GC,PAIM
COMMON/OVERFL/ OVF
COMMON/BIGNUM/ BIG
COMMON/PAI/ PI
COMMON/NTIME1/ NTIMES(14)
COMMON/NSWEEP/ NISP,NJSP,NKSP
COMMON/OUT/ IPREF,JPREK,PREK
COMMON/PEXTP/ PBCEXT

C
DATA MAXVAR,NW,NZMUT,NGAM,NRHO /14,11,12,13,14/
DATA NV,NRW,NP,NPC/1,2,3,4,5/,
& NK,NK2/6,7/
DATA CONVGN / .FALSE. /
DATA ONCE / .TRUE. /
CINI DATA TITLE/14*' /
DATA CONTMX,CONTOT,RESMAX/0.,0.,14*0./
DATA TIME,ITER/0.,0./
CINI DATA RELAX,RELSOR/14*1.,14*1./
DATA NTIMES/14*1/
DATA NISP,NJSP,NKSP/3*2/
DATA DT,OVFLW,BIG/1.E20,1.E-30,1.E30/
DATA PI/3.1415926/
C
DATA R(1)/0.0/
DATA SIMPLE / .TRUE. /
C
DATA RHOVAR/ .FALSE. /
DATA UNIFORM/ .FALSE. /
DATA NOTURB/ .FALSE. /
DATA NSOLST /1/
DATA SOLVE/ .TRUE. , .TRUE. , .TRUE. , .FALSE. , .TRUE. ,
& .TRUE. , .TRUE. , .FALSE. , .FALSE. , .FALSE. ,
& .FALSE., .FALSE., .FALSE., .FALSE., .FALSE.,
DATA (RELAX(I), I=1,3) / 0.35, 0.45, 0.40/
DATA RELAX(4) / 0.40/
DATA (RELAX(I), I=6,7) / 0.40, 0.40/
DATA RELAX(13) / 1.0/
C --------- CHANGE UNDER-RELAXATION FACTORS FOR VAR'S -----
DATA (ITRLAX(I), I=1,9) / 40, 80, 120, 160, 200, 240, 280, 320, 360/
DATA NCHNGE / 9, 9, 9, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0/
C --------- DBETA(NCHNGE(NVAR), NVAR) ---------
DATA (DBETA(I,1), I=1,9) / 9* 0.05/
DATA (DBETA(I,2), I=1,9) / 9* 0.05/
DATA (DBETA(I,3), I=1,9) / 9* 0.05/
DATA (DBETA(I,4), I=1,9) / 9* 0.05/
DATA (DBETA(I,6), I=1,9) / 9* 0.05/
DATA (DBETA(I,7), I=1,9) / 9* 0.05/
DATA (RELSOR(I), I=1,3) / 0.6, 0.6, 0.6/
DATA (RELSOR(I), I=6,7) / 0.6, 0.6/
DATA (DTLAX(I), I=1,3) / 3* 1.E30/
DATA (DTLAX(I), I=6,7) / 2* 1.E30/
C
DATA PRNT / .TRUE., .TRUE., .TRUE., .FALSE., .FALSE.,
& .TRUE., .TRUE., .FALSE., .FALSE., .FALSE., .FALSE.,
& .FALSE., .FALSE., .FALSE., .FALSE., .FALSE., .FALSE.,
& .TRUE., .TRUE., .FALSE., .FALSE., .FALSE.,
& .FALSE., .FALSE., .FALSE., .FALSE., .FALSE., .FALSE.,
DATA (TITLE(I), I=1,2) / 'V, radial (m/s)', 'W, swirl (m/s) '/
DATA (TITLE(I), I=3,3) / 'U, axial (m/s) '/
DATA (TITLE(I), I=4,5) / 'Pressure', 'Stream Function' '/
DATA (TITLE(I), I=6,7) / 'Kinetic Energy', 'Dissipatn Rate' '/
DATA (TITLE(I), I=11,12) / 'Kinematic Visco', 'Kinem Turb Visc' '/
DATA GZ, GC/ 32.174, 32.174/ , PATM/ 2116.2/
DATA RHOCON/ 62.4/, ZMUL/ 0.0033598/
DATA XL, YL, ZL/ 11.5, 5.75, 92.0/
DATA DIMPHEL/ 4.0/, RPM/ 200.0/
DATA JBAFFL/ 17/
DATA VIBC/ 42.79, 83.87, 117.97, 126.63, 105.29, 60.73/
DATA WIBC/ 92.23, 178.87, 250.03, 268.01, 223.63, 130.21/
DATA UIBC/ 57.85, 52.33, 37.52, 12.08, -20.71, -47.48, -55.62/
DATA IPT, JPT, KPT/ 30, 23, 25/, IPREF, JPREF, KPREF/ 30, 23, 25/
DATA PBCEXT/ .TRUE./
DATA LAST/ 999/
END
Appendix D:

A Sample Output

This appendix gives the locations of grid points and control faces in the finite domain scheme. A typical set of simulation results is also included here.
GRID OF TANK SYSTEM 1

<table>
<thead>
<tr>
<th>I</th>
<th>XU(I)</th>
<th>X(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>---</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>0.000</td>
<td>0.120</td>
</tr>
<tr>
<td>3</td>
<td>0.240</td>
<td>0.295</td>
</tr>
<tr>
<td>4</td>
<td>0.350</td>
<td>0.500</td>
</tr>
<tr>
<td>5</td>
<td>0.650</td>
<td>0.763</td>
</tr>
<tr>
<td>6</td>
<td>0.875</td>
<td>1.250</td>
</tr>
<tr>
<td>7</td>
<td>1.625</td>
<td>2.000</td>
</tr>
<tr>
<td>8</td>
<td>2.375</td>
<td>2.750</td>
</tr>
<tr>
<td>9</td>
<td>3.125</td>
<td>3.500</td>
</tr>
<tr>
<td>10</td>
<td>3.875</td>
<td>4.250</td>
</tr>
<tr>
<td>11</td>
<td>4.625</td>
<td>5.000</td>
</tr>
<tr>
<td>12</td>
<td>5.375</td>
<td>5.412</td>
</tr>
<tr>
<td>13</td>
<td>5.450</td>
<td>5.500</td>
</tr>
<tr>
<td>14</td>
<td>5.550</td>
<td>5.600</td>
</tr>
<tr>
<td>15</td>
<td>5.650</td>
<td>5.700</td>
</tr>
<tr>
<td>16</td>
<td>5.750</td>
<td>5.800</td>
</tr>
<tr>
<td>17</td>
<td>5.850</td>
<td>5.900</td>
</tr>
<tr>
<td>18</td>
<td>5.950</td>
<td>6.000</td>
</tr>
<tr>
<td>19</td>
<td>6.050</td>
<td>6.088</td>
</tr>
<tr>
<td>20</td>
<td>6.125</td>
<td>6.500</td>
</tr>
<tr>
<td>21</td>
<td>6.875</td>
<td>7.250</td>
</tr>
<tr>
<td>22</td>
<td>7.625</td>
<td>8.000</td>
</tr>
<tr>
<td>23</td>
<td>8.375</td>
<td>8.750</td>
</tr>
<tr>
<td>24</td>
<td>9.125</td>
<td>9.500</td>
</tr>
<tr>
<td>25</td>
<td>9.875</td>
<td>10.250</td>
</tr>
<tr>
<td>26</td>
<td>10.625</td>
<td>10.738</td>
</tr>
<tr>
<td>27</td>
<td>10.850</td>
<td>11.000</td>
</tr>
<tr>
<td>28</td>
<td>11.150</td>
<td>11.205</td>
</tr>
<tr>
<td>29</td>
<td>11.260</td>
<td>11.380</td>
</tr>
<tr>
<td>30</td>
<td>11.500</td>
<td>11.500</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>J</th>
<th>YV(J)</th>
<th>Y(J)</th>
<th>YW(J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>---</td>
<td>0.000</td>
<td>5.750</td>
</tr>
<tr>
<td>2</td>
<td>0.000</td>
<td>0.125</td>
<td>5.625</td>
</tr>
<tr>
<td>3</td>
<td>0.250</td>
<td>0.375</td>
<td>5.375</td>
</tr>
<tr>
<td>4</td>
<td>0.500</td>
<td>0.625</td>
<td>5.125</td>
</tr>
<tr>
<td>5</td>
<td>0.750</td>
<td>0.875</td>
<td>4.875</td>
</tr>
<tr>
<td>6</td>
<td>1.000</td>
<td>1.125</td>
<td>4.625</td>
</tr>
<tr>
<td>7</td>
<td>1.250</td>
<td>1.350</td>
<td>4.400</td>
</tr>
<tr>
<td>8</td>
<td>1.450</td>
<td>1.475</td>
<td>4.275</td>
</tr>
<tr>
<td>9</td>
<td>1.500</td>
<td>1.525</td>
<td>4.225</td>
</tr>
<tr>
<td>10</td>
<td>1.550</td>
<td>1.605</td>
<td>4.145</td>
</tr>
<tr>
<td>11</td>
<td>1.660</td>
<td>1.750</td>
<td>4.000</td>
</tr>
<tr>
<td>12</td>
<td>1.840</td>
<td>1.940</td>
<td>3.810</td>
</tr>
<tr>
<td>13</td>
<td>2.040</td>
<td>2.190</td>
<td>3.560</td>
</tr>
<tr>
<td>14</td>
<td>2.340</td>
<td>2.500</td>
<td>3.250</td>
</tr>
<tr>
<td>15</td>
<td>2.660</td>
<td>2.705</td>
<td>3.045</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>----</td>
<td>----</td>
<td>----</td>
</tr>
<tr>
<td>16</td>
<td>2.750</td>
<td>3.000</td>
<td>2.750</td>
</tr>
<tr>
<td>17</td>
<td>3.250</td>
<td>3.500</td>
<td>2.250</td>
</tr>
<tr>
<td>18</td>
<td>3.750</td>
<td>4.000</td>
<td>1.750</td>
</tr>
<tr>
<td>19</td>
<td>4.250</td>
<td>4.500</td>
<td>1.250</td>
</tr>
<tr>
<td>20</td>
<td>4.750</td>
<td>4.845</td>
<td>0.905</td>
</tr>
<tr>
<td>21</td>
<td>4.940</td>
<td>5.000</td>
<td>0.750</td>
</tr>
<tr>
<td>22</td>
<td>5.060</td>
<td>5.190</td>
<td>0.560</td>
</tr>
<tr>
<td>23</td>
<td>5.320</td>
<td>5.440</td>
<td>0.310</td>
</tr>
<tr>
<td>24</td>
<td>5.560</td>
<td>5.624</td>
<td>0.126</td>
</tr>
<tr>
<td>25</td>
<td>5.688</td>
<td>5.719</td>
<td>0.031</td>
</tr>
<tr>
<td>26</td>
<td>5.750</td>
<td>5.750</td>
<td>0.000</td>
</tr>
</tbody>
</table>

K

<table>
<thead>
<tr>
<th></th>
<th>ZW(K)</th>
<th>Z(K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>---</td>
<td>-1.000</td>
</tr>
<tr>
<td>2</td>
<td>-1.000</td>
<td>-0.500</td>
</tr>
<tr>
<td>3</td>
<td>0.000</td>
<td>0.500</td>
</tr>
<tr>
<td>4</td>
<td>1.000</td>
<td>2.000</td>
</tr>
<tr>
<td>5</td>
<td>3.000</td>
<td>4.000</td>
</tr>
<tr>
<td>6</td>
<td>5.000</td>
<td>6.500</td>
</tr>
<tr>
<td>7</td>
<td>8.000</td>
<td>9.500</td>
</tr>
<tr>
<td>8</td>
<td>11.000</td>
<td>12.500</td>
</tr>
<tr>
<td>9</td>
<td>14.000</td>
<td>15.500</td>
</tr>
<tr>
<td>10</td>
<td>17.000</td>
<td>19.000</td>
</tr>
<tr>
<td>11</td>
<td>21.000</td>
<td>25.500</td>
</tr>
<tr>
<td>12</td>
<td>30.000</td>
<td>35.000</td>
</tr>
<tr>
<td>13</td>
<td>40.000</td>
<td>45.000</td>
</tr>
<tr>
<td>14</td>
<td>50.000</td>
<td>55.000</td>
</tr>
<tr>
<td>15</td>
<td>60.000</td>
<td>64.500</td>
</tr>
<tr>
<td>16</td>
<td>69.000</td>
<td>71.000</td>
</tr>
<tr>
<td>17</td>
<td>73.000</td>
<td>74.500</td>
</tr>
<tr>
<td>18</td>
<td>76.000</td>
<td>77.500</td>
</tr>
<tr>
<td>19</td>
<td>79.000</td>
<td>80.500</td>
</tr>
<tr>
<td>20</td>
<td>82.000</td>
<td>83.500</td>
</tr>
<tr>
<td>21</td>
<td>85.000</td>
<td>86.000</td>
</tr>
<tr>
<td>22</td>
<td>87.000</td>
<td>88.000</td>
</tr>
<tr>
<td>23</td>
<td>89.000</td>
<td>89.500</td>
</tr>
<tr>
<td>24</td>
<td>90.000</td>
<td>90.500</td>
</tr>
<tr>
<td>25</td>
<td>91.000</td>
<td>91.000</td>
</tr>
</tbody>
</table>

GRID OF TANK SYSTEM 2

<table>
<thead>
<tr>
<th></th>
<th>XU(I)</th>
<th>X(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>---</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>0.000</td>
<td>0.120</td>
</tr>
<tr>
<td>3</td>
<td>0.240</td>
<td>0.295</td>
</tr>
<tr>
<td>4</td>
<td>0.350</td>
<td>0.500</td>
</tr>
<tr>
<td>5</td>
<td>0.650</td>
<td>0.763</td>
</tr>
<tr>
<td>6</td>
<td>0.875</td>
<td>1.250</td>
</tr>
<tr>
<td>7</td>
<td>1.625</td>
<td>2.000</td>
</tr>
<tr>
<td>J</td>
<td>YV(J)</td>
<td>Y(J)</td>
</tr>
<tr>
<td>----</td>
<td>-------</td>
<td>------</td>
</tr>
<tr>
<td>1</td>
<td>---</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>0.000</td>
<td>0.188</td>
</tr>
<tr>
<td>3</td>
<td>0.375</td>
<td>0.563</td>
</tr>
<tr>
<td>4</td>
<td>0.750</td>
<td>0.938</td>
</tr>
<tr>
<td>5</td>
<td>1.125</td>
<td>1.313</td>
</tr>
<tr>
<td>6</td>
<td>1.500</td>
<td>1.688</td>
</tr>
<tr>
<td>7</td>
<td>1.875</td>
<td>1.913</td>
</tr>
<tr>
<td>8</td>
<td>1.950</td>
<td>1.975</td>
</tr>
<tr>
<td>9</td>
<td>2.000</td>
<td>2.020</td>
</tr>
<tr>
<td>10</td>
<td>2.040</td>
<td>2.120</td>
</tr>
<tr>
<td>11</td>
<td>2.200</td>
<td>2.285</td>
</tr>
<tr>
<td>12</td>
<td>2.370</td>
<td>2.620</td>
</tr>
<tr>
<td>13</td>
<td>2.870</td>
<td>3.120</td>
</tr>
<tr>
<td>14</td>
<td>3.370</td>
<td>3.620</td>
</tr>
<tr>
<td>15</td>
<td>3.870</td>
<td>4.000</td>
</tr>
<tr>
<td>16</td>
<td>4.130</td>
<td>4.500</td>
</tr>
<tr>
<td>17</td>
<td>4.870</td>
<td>4.975</td>
</tr>
<tr>
<td>18</td>
<td>5.080</td>
<td>5.190</td>
</tr>
<tr>
<td>19</td>
<td>5.300</td>
<td>5.350</td>
</tr>
<tr>
<td>20</td>
<td>5.400</td>
<td>5.500</td>
</tr>
<tr>
<td>21</td>
<td>5.600</td>
<td>5.644</td>
</tr>
<tr>
<td>22</td>
<td>5.688</td>
<td>5.719</td>
</tr>
<tr>
<td>23</td>
<td>5.750</td>
<td>5.750</td>
</tr>
<tr>
<td>K</td>
<td>ZW(K)</td>
<td>Z(K)</td>
</tr>
<tr>
<td>----</td>
<td>-------</td>
<td>------</td>
</tr>
<tr>
<td>1</td>
<td>---</td>
<td>-1.000</td>
</tr>
<tr>
<td>I</td>
<td>XU(I)</td>
<td>X(I)</td>
</tr>
<tr>
<td>----</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>1</td>
<td>---</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>0.000</td>
<td>0.120</td>
</tr>
<tr>
<td>3</td>
<td>0.240</td>
<td>0.295</td>
</tr>
<tr>
<td>4</td>
<td>0.350</td>
<td>0.500</td>
</tr>
<tr>
<td>5</td>
<td>0.650</td>
<td>0.763</td>
</tr>
<tr>
<td>6</td>
<td>0.875</td>
<td>1.250</td>
</tr>
<tr>
<td>7</td>
<td>1.625</td>
<td>2.000</td>
</tr>
<tr>
<td>8</td>
<td>2.375</td>
<td>2.750</td>
</tr>
<tr>
<td>9</td>
<td>3.125</td>
<td>3.500</td>
</tr>
<tr>
<td>10</td>
<td>3.875</td>
<td>4.250</td>
</tr>
<tr>
<td>11</td>
<td>4.625</td>
<td>4.950</td>
</tr>
<tr>
<td>12</td>
<td>5.275</td>
<td>5.313</td>
</tr>
<tr>
<td>13</td>
<td>5.350</td>
<td>5.425</td>
</tr>
<tr>
<td>14</td>
<td>5.500</td>
<td>5.575</td>
</tr>
<tr>
<td>15</td>
<td>5.650</td>
<td>5.700</td>
</tr>
<tr>
<td>16</td>
<td>5.750</td>
<td>5.800</td>
</tr>
<tr>
<td>17</td>
<td>5.850</td>
<td>5.925</td>
</tr>
<tr>
<td>18</td>
<td>6.000</td>
<td>6.075</td>
</tr>
<tr>
<td>19</td>
<td>6.150</td>
<td>6.188</td>
</tr>
<tr>
<td>20</td>
<td>6.225</td>
<td>6.550</td>
</tr>
<tr>
<td>21</td>
<td>6.875</td>
<td>7.250</td>
</tr>
<tr>
<td>22</td>
<td>7.625</td>
<td>8.000</td>
</tr>
<tr>
<td>23</td>
<td>8.375</td>
<td>8.750</td>
</tr>
<tr>
<td>J</td>
<td>YV(J)</td>
<td>Y(J)</td>
</tr>
<tr>
<td>----</td>
<td>-------</td>
<td>------</td>
</tr>
<tr>
<td>1</td>
<td>---</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>0.000</td>
<td>0.188</td>
</tr>
<tr>
<td>3</td>
<td>0.375</td>
<td>0.563</td>
</tr>
<tr>
<td>4</td>
<td>0.750</td>
<td>0.938</td>
</tr>
<tr>
<td>5</td>
<td>1.125</td>
<td>1.313</td>
</tr>
<tr>
<td>6</td>
<td>1.500</td>
<td>1.688</td>
</tr>
<tr>
<td>7</td>
<td>1.875</td>
<td>1.913</td>
</tr>
<tr>
<td>8</td>
<td>1.950</td>
<td>1.975</td>
</tr>
<tr>
<td>9</td>
<td>2.000</td>
<td>2.020</td>
</tr>
<tr>
<td>10</td>
<td>2.040</td>
<td>2.190</td>
</tr>
<tr>
<td>11</td>
<td>2.340</td>
<td>2.500</td>
</tr>
<tr>
<td>12</td>
<td>2.660</td>
<td>2.705</td>
</tr>
<tr>
<td>13</td>
<td>2.750</td>
<td>3.000</td>
</tr>
<tr>
<td>14</td>
<td>3.250</td>
<td>3.500</td>
</tr>
<tr>
<td>15</td>
<td>3.750</td>
<td>4.000</td>
</tr>
<tr>
<td>16</td>
<td>4.250</td>
<td>4.500</td>
</tr>
<tr>
<td>17</td>
<td>4.750</td>
<td>4.845</td>
</tr>
<tr>
<td>18</td>
<td>4.940</td>
<td>5.000</td>
</tr>
<tr>
<td>19</td>
<td>5.060</td>
<td>5.190</td>
</tr>
<tr>
<td>20</td>
<td>5.320</td>
<td>5.440</td>
</tr>
<tr>
<td>21</td>
<td>5.560</td>
<td>5.624</td>
</tr>
<tr>
<td>22</td>
<td>5.688</td>
<td>5.719</td>
</tr>
<tr>
<td>23</td>
<td>5.750</td>
<td>5.750</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>K</th>
<th>ZW(K)</th>
<th>Z(K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>---</td>
<td>-1.000</td>
</tr>
<tr>
<td>2</td>
<td>-1.000</td>
<td>-0.500</td>
</tr>
<tr>
<td>3</td>
<td>0.000</td>
<td>0.500</td>
</tr>
<tr>
<td>4</td>
<td>1.000</td>
<td>2.000</td>
</tr>
<tr>
<td>5</td>
<td>3.000</td>
<td>4.000</td>
</tr>
<tr>
<td>6</td>
<td>5.000</td>
<td>6.500</td>
</tr>
<tr>
<td>7</td>
<td>8.000</td>
<td>9.500</td>
</tr>
<tr>
<td>8</td>
<td>11.000</td>
<td>12.500</td>
</tr>
<tr>
<td>9</td>
<td>14.000</td>
<td>15.500</td>
</tr>
<tr>
<td>10</td>
<td>17.000</td>
<td>19.000</td>
</tr>
<tr>
<td>11</td>
<td>21.000</td>
<td>25.500</td>
</tr>
<tr>
<td>12</td>
<td>30.000</td>
<td>35.000</td>
</tr>
<tr>
<td>13</td>
<td>40.000</td>
<td>45.000</td>
</tr>
<tr>
<td>14</td>
<td>50.000</td>
<td>55.000</td>
</tr>
<tr>
<td>15</td>
<td>60.000</td>
<td>64.500</td>
</tr>
<tr>
<td>16</td>
<td>69.000</td>
<td>71.000</td>
</tr>
<tr>
<td>17</td>
<td>73.000</td>
<td>74.500</td>
</tr>
</tbody>
</table>
FLOW FIELD MODELING IN TANK SYSTEM 3

THE FOLLOWING TABULATED VALUES ARE IN SI UNIT

<table>
<thead>
<tr>
<th>I=</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>J=</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>22</td>
<td>0.0000+000</td>
<td>-2.7013-003</td>
<td>-3.0907-003</td>
<td>-2.6452-003</td>
<td>-2.2601-003</td>
<td>-2.4910-003</td>
</tr>
<tr>
<td>21</td>
<td>0.0000+000</td>
<td>-1.1329-002</td>
<td>-1.2466-002</td>
<td>-1.1516-002</td>
<td>-1.0193-002</td>
<td>-1.0260-002</td>
</tr>
<tr>
<td>20</td>
<td>0.0000+000</td>
<td>-2.9072-002</td>
<td>-3.0269-002</td>
<td>-2.9580-002</td>
<td>-2.7418-002</td>
<td>-2.5936-002</td>
</tr>
<tr>
<td>19</td>
<td>0.0000+000</td>
<td>-5.3807-002</td>
<td>-5.4503-002</td>
<td>-5.4234-002</td>
<td>-5.1578-002</td>
<td>-4.7785-002</td>
</tr>
<tr>
<td>16</td>
<td>0.0000+000</td>
<td>-1.1239-001</td>
<td>-1.1241-001</td>
<td>-1.1144-001</td>
<td>-1.0705-001</td>
<td>-9.8442-002</td>
</tr>
<tr>
<td>15</td>
<td>0.0000+000</td>
<td>-1.2489-001</td>
<td>-1.2376-001</td>
<td>-1.2160-001</td>
<td>-1.1649-001</td>
<td>-1.0893-001</td>
</tr>
<tr>
<td>14</td>
<td>0.0000+000</td>
<td>-1.2722-001</td>
<td>-1.2508-001</td>
<td>-1.2192-001</td>
<td>-1.1622-001</td>
<td>-1.0803-001</td>
</tr>
<tr>
<td>13</td>
<td>0.0000+000</td>
<td>-1.2087-001</td>
<td>-1.1880-001</td>
<td>-1.1519-001</td>
<td>-1.0931-001</td>
<td>-9.9717-002</td>
</tr>
<tr>
<td>12</td>
<td>0.0000+000</td>
<td>-1.1485-001</td>
<td>-1.1244-001</td>
<td>-1.0906-001</td>
<td>-1.0339-001</td>
<td>-9.3113-002</td>
</tr>
<tr>
<td>11</td>
<td>0.0000+000</td>
<td>-1.0791-001</td>
<td>-1.0496-001</td>
<td>-1.0175-001</td>
<td>-9.6597-002</td>
<td>-8.6557-002</td>
</tr>
<tr>
<td>6</td>
<td>0.0000+000</td>
<td>-6.6229-002</td>
<td>-6.4610-002</td>
<td>-6.2734-002</td>
<td>-6.0039-002</td>
<td>-5.3898-002</td>
</tr>
<tr>
<td>5</td>
<td>0.0000+000</td>
<td>-4.6616-002</td>
<td>-4.5750-002</td>
<td>-4.4624-002</td>
<td>-4.2934-002</td>
<td>-3.9077-002</td>
</tr>
<tr>
<td>4</td>
<td>0.0000+000</td>
<td>-3.0370-002</td>
<td>-2.9903-002</td>
<td>-2.9303-002</td>
<td>-2.8358-002</td>
<td>-2.6282-002</td>
</tr>
<tr>
<td>3</td>
<td>0.0000+000</td>
<td>-1.6746-002</td>
<td>-1.6431-002</td>
<td>-1.6138-002</td>
<td>-1.5736-002</td>
<td>-1.4910-002</td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>-5.2364-003</td>
<td>-5.0860-003</td>
<td>-4.9914-003</td>
<td>-4.9073-003</td>
<td>-4.7462-003</td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>I=</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>J=</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>22</td>
<td>-2.4655-003</td>
<td>-2.4756-003</td>
<td>-2.3882-003</td>
<td>-1.7241-003</td>
<td>5.7781-004</td>
<td>4.2895-003</td>
</tr>
<tr>
<td>21</td>
<td>-1.0064-002</td>
<td>-1.0112-002</td>
<td>-9.7222-003</td>
<td>-6.9110-003</td>
<td>2.6640-003</td>
<td>1.5799-002</td>
</tr>
<tr>
<td>J=</td>
<td>13</td>
<td>14</td>
<td>15</td>
<td>16</td>
<td>17</td>
<td>18</td>
</tr>
<tr>
<td>-----</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
</tr>
<tr>
<td>23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>22</td>
<td>4.1649-003</td>
<td>4.8356-003</td>
<td>5.1654-003</td>
<td>5.2761-003</td>
<td>5.1798-003</td>
<td>4.7008-003</td>
</tr>
<tr>
<td>21</td>
<td>1.7187-002</td>
<td>1.9626-002</td>
<td>2.0799-002</td>
<td>2.1158-002</td>
<td>2.0792-002</td>
<td>1.8971-002</td>
</tr>
<tr>
<td>18</td>
<td>9.3106-002</td>
<td>1.1318-001</td>
<td>1.2035-001</td>
<td>1.2284-001</td>
<td>1.2158-001</td>
<td>1.1122-001</td>
</tr>
<tr>
<td>17</td>
<td>9.9673-002</td>
<td>1.1662-001</td>
<td>1.2480-001</td>
<td>1.2781-001</td>
<td>1.2684-001</td>
<td>1.1599-001</td>
</tr>
<tr>
<td>16</td>
<td>1.6463-001</td>
<td>1.9038-001</td>
<td>2.0346-001</td>
<td>2.0903-001</td>
<td>2.0944-001</td>
<td>1.9624-001</td>
</tr>
<tr>
<td>15</td>
<td>2.8244-001</td>
<td>3.2221-001</td>
<td>3.4289-001</td>
<td>3.5215-001</td>
<td>3.5395-001</td>
<td>3.3582-001</td>
</tr>
<tr>
<td>14</td>
<td>3.6019-001</td>
<td>4.1342-001</td>
<td>4.4118-001</td>
<td>4.5314-001</td>
<td>4.5408-001</td>
<td>4.2741-001</td>
</tr>
<tr>
<td>13</td>
<td>3.9615-001</td>
<td>4.7157-001</td>
<td>5.1204-001</td>
<td>5.2747-001</td>
<td>5.2272-001</td>
<td>4.7433-001</td>
</tr>
<tr>
<td>12</td>
<td>3.9878-001</td>
<td>4.9536-001</td>
<td>5.4971-001</td>
<td>5.6856-001</td>
<td>5.5933-001</td>
<td>4.8311-001</td>
</tr>
<tr>
<td>11</td>
<td>3.6751-001</td>
<td>4.9778-001</td>
<td>5.8159-001</td>
<td>6.0746-001</td>
<td>5.7460-001</td>
<td>4.5782-001</td>
</tr>
<tr>
<td>10</td>
<td>2.8083-001</td>
<td>4.6810-001</td>
<td>6.2271-001</td>
<td>6.6753-001</td>
<td>5.7444-001</td>
<td>3.7494-001</td>
</tr>
<tr>
<td>9</td>
<td>2.1894-001</td>
<td>4.3181-001</td>
<td>6.1901-001</td>
<td>6.6996-001</td>
<td>5.4758-001</td>
<td>3.1094-001</td>
</tr>
<tr>
<td>8</td>
<td>2.0204-001</td>
<td>4.3775-001</td>
<td>5.9518-001</td>
<td>6.4640-001</td>
<td>5.4738-001</td>
<td>2.7366-001</td>
</tr>
<tr>
<td>7</td>
<td>1.6778-001</td>
<td>4.4896-001</td>
<td>5.8212-001</td>
<td>6.3012-001</td>
<td>5.5824-001</td>
<td>2.1155-001</td>
</tr>
<tr>
<td>6</td>
<td>1.3301-001</td>
<td>3.9293-001</td>
<td>5.3040-001</td>
<td>5.6578-001</td>
<td>4.8551-001</td>
<td>1.6503-001</td>
</tr>
<tr>
<td>5</td>
<td>9.8205-002</td>
<td>2.6401-001</td>
<td>4.1735-001</td>
<td>4.5097-001</td>
<td>3.3440-001</td>
<td>1.2189-001</td>
</tr>
<tr>
<td>4</td>
<td>6.6798-002</td>
<td>1.4467-001</td>
<td>2.8212-001</td>
<td>3.1820-001</td>
<td>2.0567-001</td>
<td>8.0342-002</td>
</tr>
<tr>
<td>3</td>
<td>2.7174-002</td>
<td>4.9343-002</td>
<td>1.0858-001</td>
<td>1.2765-001</td>
<td>7.8489-002</td>
<td>3.1354-002</td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>I=</th>
<th>19</th>
<th>20</th>
<th>21</th>
<th>22</th>
<th>23</th>
<th>24</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>22</td>
<td>4.8794-003</td>
<td>8.4122-004</td>
<td>1.7168-003</td>
<td>2.4694-003</td>
<td>2.6160-003</td>
<td>2.6702-003</td>
</tr>
<tr>
<td>16</td>
<td>1.7568-001</td>
<td>2.8962-002</td>
<td>8.1157-002</td>
<td>1.0484-001</td>
<td>1.0456-001</td>
<td>1.0089-001</td>
</tr>
<tr>
<td>J</td>
<td>20</td>
<td>21</td>
<td>22</td>
<td>23</td>
<td>24</td>
<td>25</td>
</tr>
<tr>
<td>----</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
</tr>
<tr>
<td>14</td>
<td>3.8917-001</td>
<td>1.1022-001</td>
<td>-9.1333-002</td>
<td>-1.3446-001</td>
<td>-1.3378-001</td>
<td>-1.2455-001</td>
</tr>
<tr>
<td>3</td>
<td>2.5835-002</td>
<td>1.4389-002</td>
<td>-1.9654-003</td>
<td>-6.7576-003</td>
<td>-7.9598-003</td>
<td>-8.3652-003</td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>J=</td>
<td>I=</td>
<td>7</td>
<td>8</td>
<td>9</td>
<td>10</td>
<td>11</td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>-----------</td>
<td>-----------</td>
<td>-----------</td>
<td>-----------</td>
<td>-----------</td>
</tr>
<tr>
<td>22</td>
<td>-2.4655-003</td>
<td>-2.4756-003</td>
<td>-2.3882-003</td>
<td>-1.7241-003</td>
<td>5.7781-004</td>
<td>4.2895-003</td>
</tr>
<tr>
<td>21</td>
<td>-1.0064-002</td>
<td>-1.0112-002</td>
<td>-9.7222-003</td>
<td>-6.9110-003</td>
<td>2.6640-003</td>
<td>1.5799-002</td>
</tr>
<tr>
<td>14</td>
<td>-1.0827-001</td>
<td>-1.1631-001</td>
<td>-1.1724-001</td>
<td>-7.9745-002</td>
<td>8.9373-002</td>
<td>3.1021-001</td>
</tr>
<tr>
<td>8</td>
<td>-5.9857-002</td>
<td>-5.5419-002</td>
<td>-4.2968-002</td>
<td>-1.1239-002</td>
<td>6.7678-002</td>
<td>1.8056-001</td>
</tr>
<tr>
<td>2</td>
<td>-4.4066-003</td>
<td>-3.7470-003</td>
<td>-1.7680-003</td>
<td>3.6035-003</td>
<td>1.7140-002</td>
<td>1.5596-002</td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>J=</th>
<th>I=</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>23</td>
</tr>
<tr>
<td>22</td>
<td>4.1649-003</td>
<td>4.8356-003</td>
<td>5.1654-003</td>
<td>5.2761-003</td>
<td>5.1798-003</td>
<td>4.7008-003</td>
<td>22</td>
</tr>
<tr>
<td>21</td>
<td>1.7187-002</td>
<td>1.9626-002</td>
<td>2.0799-002</td>
<td>2.1158-002</td>
<td>2.0792-002</td>
<td>1.8971-002</td>
<td>21</td>
</tr>
<tr>
<td>18</td>
<td>9.8106-002</td>
<td>1.1318-001</td>
<td>1.2035-001</td>
<td>1.2284-001</td>
<td>1.2158-001</td>
<td>1.1122-001</td>
<td>18</td>
</tr>
<tr>
<td>17</td>
<td>9.9673-002</td>
<td>1.1662-001</td>
<td>1.2480-001</td>
<td>1.2781-001</td>
<td>1.2684-001</td>
<td>1.1599-001</td>
<td>17</td>
</tr>
<tr>
<td>16</td>
<td>1.6463-001</td>
<td>1.9038-001</td>
<td>2.0346-001</td>
<td>2.0903-001</td>
<td>2.0944-001</td>
<td>1.9624-001</td>
<td>16</td>
</tr>
<tr>
<td>I=</td>
<td>19</td>
<td>20</td>
<td>21</td>
<td>22</td>
<td>23</td>
<td>24</td>
<td>J=</td>
</tr>
<tr>
<td>-----</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>------</td>
</tr>
<tr>
<td>14</td>
<td>3.6019-001</td>
<td>4.1342-001</td>
<td>4.4118-001</td>
<td>4.5314-001</td>
<td>4.5408-001</td>
<td>4.2741-001</td>
<td>14</td>
</tr>
<tr>
<td>13</td>
<td>3.9615-001</td>
<td>4.7157-001</td>
<td>5.1204-001</td>
<td>5.2747-001</td>
<td>5.2272-001</td>
<td>4.7433-001</td>
<td>13</td>
</tr>
<tr>
<td>12</td>
<td>3.9878-001</td>
<td>4.9536-001</td>
<td>5.4971-001</td>
<td>5.6856-001</td>
<td>5.5593-001</td>
<td>4.8311-001</td>
<td>12</td>
</tr>
<tr>
<td>11</td>
<td>3.6751-001</td>
<td>4.9778-001</td>
<td>5.8155-001</td>
<td>6.0746-001</td>
<td>5.7460-001</td>
<td>4.5782-001</td>
<td>11</td>
</tr>
<tr>
<td>10</td>
<td>2.8083-001</td>
<td>4.6810-001</td>
<td>6.2271-001</td>
<td>6.6753-001</td>
<td>5.7444-001</td>
<td>3.7494-001</td>
<td>10</td>
</tr>
<tr>
<td>9</td>
<td>2.1894-001</td>
<td>4.3181-001</td>
<td>6.1901-001</td>
<td>6.6996-001</td>
<td>5.4758-001</td>
<td>3.1094-001</td>
<td>9</td>
</tr>
<tr>
<td>8</td>
<td>2.0204-001</td>
<td>4.3775-001</td>
<td>5.9518-001</td>
<td>6.4640-001</td>
<td>5.4738-001</td>
<td>2.7366-001</td>
<td>8</td>
</tr>
<tr>
<td>7</td>
<td>1.6778-001</td>
<td>4.4896-001</td>
<td>5.8212-001</td>
<td>6.3012-001</td>
<td>5.5824-001</td>
<td>2.1155-001</td>
<td>7</td>
</tr>
<tr>
<td>6</td>
<td>1.3301-001</td>
<td>3.9293-001</td>
<td>5.3040-001</td>
<td>5.6578-001</td>
<td>4.8551-001</td>
<td>1.6503-001</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
<td>9.8205-002</td>
<td>2.6401-001</td>
<td>4.1735-001</td>
<td>4.5097-001</td>
<td>3.3440-001</td>
<td>1.2189-001</td>
<td>5</td>
</tr>
<tr>
<td>4</td>
<td>6.6798-002</td>
<td>1.4467-001</td>
<td>2.8212-001</td>
<td>3.1820-001</td>
<td>2.0567-001</td>
<td>8.0342-002</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>2.7174-002</td>
<td>4.9343-002</td>
<td>1.0858-001</td>
<td>1.2765-001</td>
<td>7.8489-002</td>
<td>3.1354-002</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>1</td>
</tr>
<tr>
<td>I= 1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J= 23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>0.0000+000</td>
<td>-1.1083-002</td>
<td>-2.7056-002</td>
<td>-4.5810-002</td>
<td>-6.8106-002</td>
<td>-1.0476-001</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.0000+000</td>
<td>-1.1713-002</td>
<td>-2.8269-002</td>
<td>-4.6802-002</td>
<td>-6.9400-002</td>
<td>-1.0616-001</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>0.0000+000</td>
<td>-1.1947-002</td>
<td>-2.8940-002</td>
<td>-4.7650-002</td>
<td>-7.0185-002</td>
<td>-1.0601-001</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>0.0000+000</td>
<td>-1.1950-002</td>
<td>-2.9070-002</td>
<td>-4.6885-002</td>
<td>-7.0819-002</td>
<td>-1.0556-001</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>0.0000+000</td>
<td>-1.2161-002</td>
<td>-2.9582-002</td>
<td>-4.8795-002</td>
<td>-7.1707-002</td>
<td>-1.0522-001</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0.0000+000</td>
<td>-1.3387-002</td>
<td>-3.2583-002</td>
<td>-5.2742-002</td>
<td>-7.6136-002</td>
<td>-1.0560-001</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>0.0000+000</td>
<td>-8.2804-003</td>
<td>-2.0148-002</td>
<td>-3.2478-002</td>
<td>-4.6644-002</td>
<td>-6.0892-002</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>0.0000+000</td>
<td>-3.1515-003</td>
<td>-7.7986-003</td>
<td>-1.2850-002</td>
<td>-1.8568-002</td>
<td>-2.1750-002</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>0.0000+000</td>
<td>-2.3125-003</td>
<td>-4.5867-003</td>
<td>-5.0354-003</td>
<td>-5.8797-003</td>
<td>-4.3234-003</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.0000+000</td>
<td>1.1147-003</td>
<td>2.6415-003</td>
<td>4.5767-003</td>
<td>7.2245-003</td>
<td>1.4735-002</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.0000+000</td>
<td>3.7903-003</td>
<td>9.1573-003</td>
<td>1.4958-002</td>
<td>2.2164-002</td>
<td>3.5690-002</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.0000+000</td>
<td>4.3870-003</td>
<td>1.0984-002</td>
<td>1.8607-002</td>
<td>2.7782-002</td>
<td>4.3820-002</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.0000+000</td>
<td>4.7259-003</td>
<td>1.1695-002</td>
<td>1.9665-002</td>
<td>2.9358-002</td>
<td>4.6081-002</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.0000+000</td>
<td>5.1083-003</td>
<td>1.2585-002</td>
<td>2.1058-002</td>
<td>3.1402-002</td>
<td>4.9037-002</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.0000+000</td>
<td>6.5947-003</td>
<td>1.6008-002</td>
<td>2.6163-002</td>
<td>3.8687-002</td>
<td>5.9603-002</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.0000+000</td>
<td>7.4032-003</td>
<td>1.8059-002</td>
<td>2.9814-002</td>
<td>4.4380-002</td>
<td>6.8553-002</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.0000+000</td>
<td>7.5431-003</td>
<td>1.8438-002</td>
<td>3.0666-002</td>
<td>4.5930-002</td>
<td>7.1673-002</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.0000+000</td>
<td>7.2194-003</td>
<td>1.7695-002</td>
<td>2.9648-002</td>
<td>4.4659-002</td>
<td>7.5588-002</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>6.6001-003</td>
<td>1.6131-002</td>
<td>2.6896-002</td>
<td>4.0511-002</td>
<td>6.4917-002</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>6.5971-003</td>
<td>1.6124-002</td>
<td>2.6885-002</td>
<td>4.0495-002</td>
<td>6.4895-002</td>
<td></td>
</tr>
</tbody>
</table>

---

**K = 1**
<table>
<thead>
<tr>
<th></th>
<th>I=</th>
<th>J=</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>-1.3405-001</td>
<td>-1.4447-001</td>
<td>-1.4766-001</td>
<td>-1.4585-001</td>
<td>-1.1969-001</td>
<td>-1.3405-001</td>
<td>16</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>-1.0832-001</td>
<td>-1.0911-002</td>
<td>-1.0674-001</td>
<td>-1.0544-002</td>
<td>-1.0717-001</td>
<td>-1.2615-002</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>-1.0297-001</td>
<td>-1.0480-002</td>
<td>-1.0307-001</td>
<td>-1.0357-002</td>
<td>-1.0356-001</td>
<td>-1.0632-002</td>
<td>14</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>-1.0076-001</td>
<td>-1.0213-001</td>
<td>-1.0232-001</td>
<td>-1.0216-002</td>
<td>-1.0226-001</td>
<td>-1.0357-002</td>
<td>13</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-9.0000+000</td>
<td>-9.0000+000</td>
<td>-9.0000+000</td>
<td>-9.0000+000</td>
<td>-9.0000+000</td>
<td>-9.0000+000</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>I=</th>
<th>J=</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>19</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>21</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>22</td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>23</td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>24</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>25</td>
<td>26</td>
<td>27</td>
<td>28</td>
<td>29</td>
<td>30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J=</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>9.4558-002</td>
<td>5.9453-002</td>
<td>3.9391-002</td>
<td>2.3636-002</td>
<td>9.6534-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>1.0155-001</td>
<td>6.6955-002</td>
<td>4.5034-002</td>
<td>2.6812-002</td>
<td>1.0847-002</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>1.0294-001</td>
<td>6.8227-002</td>
<td>4.5504-002</td>
<td>2.6847-002</td>
<td>1.0835-002</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>1.0285-001</td>
<td>6.9222-002</td>
<td>4.6149-002</td>
<td>2.7381-002</td>
<td>1.1071-002</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>1.0240-001</td>
<td>6.9612-002</td>
<td>4.6918-002</td>
<td>2.8023-002</td>
<td>1.1354-002</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>1.0198-001</td>
<td>7.0424-002</td>
<td>4.7825-002</td>
<td>2.8781-002</td>
<td>1.1692-002</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>1.0161-001</td>
<td>7.4107-002</td>
<td>5.1836-002</td>
<td>3.2199-002</td>
<td>1.3270-002</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>8.7540-002</td>
<td>6.5907-002</td>
<td>4.6552-002</td>
<td>2.9176-002</td>
<td>1.2061-002</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>6.0033-002</td>
<td>4.6246-002</td>
<td>3.2956-002</td>
<td>2.0739-002</td>
<td>8.5871-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>2.1726-002</td>
<td>1.8512-002</td>
<td>1.3421-002</td>
<td>8.5683-003</td>
<td>3.5751-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>4.0606-003</td>
<td>5.9148-003</td>
<td>4.7262-003</td>
<td>3.2334-003</td>
<td>1.3734-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>-1.5588-002</td>
<td>-8.0701-003</td>
<td>-4.9887-003</td>
<td>-2.7811-003</td>
<td>-1.1063-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>-3.7337-002</td>
<td>-2.2922-002</td>
<td>-1.5091-002</td>
<td>-8.9337-003</td>
<td>-3.6323-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>-4.5567-002</td>
<td>-2.8303-002</td>
<td>-1.8690-002</td>
<td>-1.1092-002</td>
<td>-4.5149-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>-4.7895-002</td>
<td>-2.9821-002</td>
<td>-1.9707-002</td>
<td>-1.1701-002</td>
<td>-4.7637-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>-5.0939-002</td>
<td>-3.1791-002</td>
<td>-2.1089-002</td>
<td>-1.2494-002</td>
<td>-5.0835-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>-6.2185-002</td>
<td>-3.9019-002</td>
<td>-2.5823-002</td>
<td>-1.5349-002</td>
<td>-6.2538-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>-7.3299-002</td>
<td>-4.6016-002</td>
<td>-3.0440-002</td>
<td>-1.8079-002</td>
<td>-7.3647-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>-8.0559-002</td>
<td>-5.0611-002</td>
<td>-3.3476-002</td>
<td>-1.9867-002</td>
<td>-8.0903-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>-9.0470-002</td>
<td>-5.7638-002</td>
<td>-3.7992-002</td>
<td>-2.2514-002</td>
<td>-9.1677-003</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

K = 1

PRESSURE

--- ALL PRESSURE VALUES ARE RELATIVE TO P(30,23,25) ---
<table>
<thead>
<tr>
<th>I</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>19</td>
<td>1.0237+004</td>
<td>1.3231+004</td>
<td>1.3233+004</td>
<td>1.3221+004</td>
<td>1.3198+004</td>
<td>1.2848+004</td>
</tr>
<tr>
<td>18</td>
<td>1.0237+004</td>
<td>1.3257+004</td>
<td>1.3239+004</td>
<td>1.3238+004</td>
<td>1.3219+004</td>
<td>1.2890+004</td>
</tr>
<tr>
<td>17</td>
<td>1.0237+004</td>
<td>1.3346+004</td>
<td>1.3295+004</td>
<td>1.3238+004</td>
<td>1.3219+004</td>
<td>1.2890+004</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>J</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>22</td>
<td>1.2497+004</td>
<td>1.2250+004</td>
<td>1.2080+004</td>
<td>1.2190+004</td>
<td>1.2946+004</td>
<td>1.3758+004</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>I</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.4427+003</td>
<td>1.0207+004</td>
<td>1.0164+004</td>
<td>1.0112+004</td>
<td>1.0047+004</td>
<td>9.9258+003</td>
</tr>
<tr>
<td>I</td>
<td>16</td>
<td>17</td>
<td>18</td>
<td>19</td>
<td>20</td>
<td>21</td>
</tr>
<tr>
<td>---</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
</tr>
<tr>
<td>1</td>
<td>1.2349+004</td>
<td>1.2513+004</td>
<td>1.2609+004</td>
<td>1.2654+004</td>
<td>1.2667+004</td>
<td>1.2621+004</td>
</tr>
<tr>
<td>2</td>
<td>1.2242+004</td>
<td>1.2394+004</td>
<td>1.2481+004</td>
<td>1.2524+004</td>
<td>1.2544+004</td>
<td>1.2516+004</td>
</tr>
<tr>
<td>3</td>
<td>1.2091+004</td>
<td>1.2194+004</td>
<td>1.2258+004</td>
<td>1.2293+004</td>
<td>1.2321+004</td>
<td>1.2325+004</td>
</tr>
<tr>
<td>4</td>
<td>1.1933+004</td>
<td>1.1976+004</td>
<td>1.2012+004</td>
<td>1.2041+004</td>
<td>1.2088+004</td>
<td>1.2154+004</td>
</tr>
<tr>
<td>5</td>
<td>1.1659+004</td>
<td>1.2054+004</td>
<td>1.2366+004</td>
<td>1.2487+004</td>
<td>1.2363+004</td>
<td>1.2109+004</td>
</tr>
<tr>
<td>6</td>
<td>1.1455+004</td>
<td>1.1831+004</td>
<td>1.2197+004</td>
<td>1.2296+004</td>
<td>1.2133+004</td>
<td>1.1837+004</td>
</tr>
<tr>
<td>7</td>
<td>1.0238+004</td>
<td>1.2034+004</td>
<td>1.4634+004</td>
<td>1.5375+004</td>
<td>1.3376+004</td>
<td>1.1287+004</td>
</tr>
<tr>
<td>8</td>
<td>3.9980+003</td>
<td>1.0440+004</td>
<td>2.8661+004</td>
<td>3.7789+004</td>
<td>1.8379+004</td>
<td>5.6878+003</td>
</tr>
<tr>
<td>9</td>
<td>-4.0402+005</td>
<td>-3.1430+005</td>
<td>-3.0356+005</td>
<td>-3.0320+005</td>
<td>-3.1864+005</td>
<td>-4.6965+005</td>
</tr>
<tr>
<td>10</td>
<td>-2.9679+005</td>
<td>-3.0850+005</td>
<td>-3.0400+005</td>
<td>-3.0341+005</td>
<td>-3.0758+005</td>
<td>-2.8030+005</td>
</tr>
<tr>
<td>11</td>
<td>-3.0722+005</td>
<td>-3.0700+005</td>
<td>-3.0633+005</td>
<td>-3.0634+005</td>
<td>-3.0721+005</td>
<td>-3.0739+005</td>
</tr>
<tr>
<td>15</td>
<td>8.8862+003</td>
<td>8.8489+003</td>
<td>8.8178+003</td>
<td>8.7929+003</td>
<td>8.7617+003</td>
<td>8.7244+003</td>
</tr>
<tr>
<td>16</td>
<td>8.8862+003</td>
<td>8.8489+003</td>
<td>8.8178+003</td>
<td>8.7929+003</td>
<td>8.7617+003</td>
<td>8.7244+003</td>
</tr>
<tr>
<td>17</td>
<td>I=</td>
<td>19</td>
<td>20</td>
<td>21</td>
<td>22</td>
<td>23</td>
</tr>
<tr>
<td>K = 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**KINETIC ENERGY**

<table>
<thead>
<tr>
<th>I=</th>
<th>J=</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>22</td>
<td>0.0000+000</td>
<td>1.4357+004</td>
<td>1.4583+004</td>
<td>1.4696+004</td>
<td>1.4768+004</td>
<td>1.4770+004</td>
<td>1.4823+004</td>
</tr>
<tr>
<td>21</td>
<td>0.0000+000</td>
<td>1.4354+004</td>
<td>1.4587+004</td>
<td>1.4699+004</td>
<td>1.4770+004</td>
<td>1.4823+004</td>
<td>1.4892+004</td>
</tr>
<tr>
<td>20</td>
<td>0.0000+000</td>
<td>1.4354+004</td>
<td>1.4587+004</td>
<td>1.4699+004</td>
<td>1.4770+004</td>
<td>1.4823+004</td>
<td>1.4892+004</td>
</tr>
<tr>
<td>19</td>
<td>0.0000+000</td>
<td>1.4373+004</td>
<td>1.4609+004</td>
<td>1.4720+004</td>
<td>1.4792+004</td>
<td>1.4844+004</td>
<td>1.4892+004</td>
</tr>
<tr>
<td>18</td>
<td>0.0000+000</td>
<td>1.4379+004</td>
<td>1.4612+004</td>
<td>1.4722+004</td>
<td>1.4792+004</td>
<td>1.4844+004</td>
<td>1.4892+004</td>
</tr>
<tr>
<td>17</td>
<td>0.0000+000</td>
<td>1.4388+004</td>
<td>1.4620+004</td>
<td>1.4731+004</td>
<td>1.4792+004</td>
<td>1.4844+004</td>
<td>1.4892+004</td>
</tr>
<tr>
<td>16</td>
<td>0.0000+000</td>
<td>1.4417+004</td>
<td>1.4661+004</td>
<td>1.4759+004</td>
<td>1.4792+004</td>
<td>1.4844+004</td>
<td>1.4880+004</td>
</tr>
<tr>
<td>15</td>
<td>0.0000+000</td>
<td>1.4464+004</td>
<td>1.4688+004</td>
<td>1.4792+004</td>
<td>1.4863+004</td>
<td>1.4913+004</td>
<td>1.4736+003</td>
</tr>
<tr>
<td>14</td>
<td>0.0000+000</td>
<td>1.4422+004</td>
<td>1.4630+004</td>
<td>1.4731+004</td>
<td>1.4801+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
</tr>
<tr>
<td>13</td>
<td>0.0000+000</td>
<td>1.4475+004</td>
<td>1.4673+004</td>
<td>1.4778+004</td>
<td>1.4849+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
</tr>
<tr>
<td>12</td>
<td>0.0000+000</td>
<td>1.4543+004</td>
<td>1.4630+004</td>
<td>1.4731+004</td>
<td>1.4801+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
</tr>
<tr>
<td>11</td>
<td>0.0000+000</td>
<td>1.4586+004</td>
<td>1.4630+004</td>
<td>1.4731+004</td>
<td>1.4801+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
</tr>
<tr>
<td>10</td>
<td>0.0000+000</td>
<td>1.4630+004</td>
<td>1.4696+004</td>
<td>1.4792+004</td>
<td>1.4849+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
</tr>
<tr>
<td>9</td>
<td>0.0000+000</td>
<td>1.4673+004</td>
<td>1.4731+004</td>
<td>1.4801+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.0000+000</td>
<td>1.4716+004</td>
<td>1.4778+004</td>
<td>1.4849+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.0000+000</td>
<td>1.4759+004</td>
<td>1.4812+004</td>
<td>1.4880+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.0000+000</td>
<td>1.4802+004</td>
<td>1.4855+004</td>
<td>1.4913+004</td>
<td>1.4736+003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.0000+000</td>
<td>1.4846+004</td>
<td>1.4901+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.0000+000</td>
<td>1.4889+004</td>
<td>1.4948+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.0000+000</td>
<td>1.4933+004</td>
<td>1.4998+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>1.4977+004</td>
<td>1.5063+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>1.5021+004</td>
<td>1.5112+004</td>
<td>1.4897+004</td>
<td>1.4736+003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>I= 1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>-----</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>J= 0</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
</tr>
<tr>
<td>J= 1</td>
<td>1.2903-001</td>
<td>1.2392-001</td>
<td>1.2139-001</td>
<td>1.2067-001</td>
<td>1.2142-001</td>
<td>1.2464-001</td>
<td>1.2392-001</td>
</tr>
<tr>
<td>J= 2</td>
<td>1.2637-001</td>
<td>1.2466-001</td>
<td>1.2367-001</td>
<td>1.2325-001</td>
<td>1.2321-001</td>
<td>1.2370-001</td>
<td>1.2367-001</td>
</tr>
<tr>
<td>J= 3</td>
<td>1.3052-001</td>
<td>1.2365-001</td>
<td>1.2371-001</td>
<td>1.2372-001</td>
<td>1.2364-001</td>
<td>1.2364-001</td>
<td>1.2371-001</td>
</tr>
<tr>
<td>J= 4</td>
<td>1.2503-001</td>
<td>1.2792-001</td>
<td>1.2692-001</td>
<td>1.2644-001</td>
<td>1.2630-001</td>
<td>1.2520-001</td>
<td>1.2692-001</td>
</tr>
<tr>
<td>J= 5</td>
<td>1.6645-001</td>
<td>1.6889-001</td>
<td>1.6995-001</td>
<td>1.7068-001</td>
<td>1.7113-001</td>
<td>1.7092-001</td>
<td>1.6889-001</td>
</tr>
<tr>
<td>J= 6</td>
<td>1.8940-001</td>
<td>1.8699-001</td>
<td>1.8726-001</td>
<td>1.8822-001</td>
<td>1.9042-001</td>
<td>1.9631-001</td>
<td>1.8699-001</td>
</tr>
<tr>
<td>J= 7</td>
<td>2.3935-001</td>
<td>2.4494-001</td>
<td>2.4571-001</td>
<td>2.4802-001</td>
<td>2.5359-001</td>
<td>2.6872-001</td>
<td>2.4494-001</td>
</tr>
<tr>
<td>J= 9</td>
<td>5.2199-001</td>
<td>5.2587-001</td>
<td>5.3904-001</td>
<td>5.4765-001</td>
<td>5.6049-001</td>
<td>6.0184-001</td>
<td>5.2587-001</td>
</tr>
<tr>
<td>J= 10</td>
<td>5.3719-001</td>
<td>5.3281-001</td>
<td>5.4000-001</td>
<td>5.4534-001</td>
<td>5.6005-001</td>
<td>6.1344-001</td>
<td>5.3281-001</td>
</tr>
<tr>
<td>J= 11</td>
<td>5.4734-001</td>
<td>5.7748-001</td>
<td>5.9626-001</td>
<td>5.9817-001</td>
<td>6.0523-001</td>
<td>6.2239-001</td>
<td>5.7748-001</td>
</tr>
<tr>
<td>J= 13</td>
<td>3.0735-001</td>
<td>5.2530-001</td>
<td>5.5346-001</td>
<td>5.5065-001</td>
<td>5.4784-001</td>
<td>3.5471-001</td>
<td>5.2530-001</td>
</tr>
<tr>
<td>J= 15</td>
<td>1.2678-001</td>
<td>1.9827-001</td>
<td>1.9007-001</td>
<td>1.8136-001</td>
<td>1.9921-001</td>
<td>1.5161-001</td>
<td>1.9827-001</td>
</tr>
<tr>
<td>J= 19</td>
<td>2.0000+000</td>
<td>2.0000+000</td>
<td>2.0000+000</td>
<td>2.0000+000</td>
<td>2.0000+000</td>
<td>2.0000+000</td>
<td>2.0000+000</td>
</tr>
<tr>
<td>J= 20</td>
<td>1.0000+000</td>
<td>1.0000+000</td>
<td>1.0000+000</td>
<td>1.0000+000</td>
<td>1.0000+000</td>
<td>1.0000+000</td>
<td>1.0000+000</td>
</tr>
<tr>
<td>J= 21</td>
<td>9.0000+000</td>
<td>9.0000+000</td>
<td>9.0000+000</td>
<td>9.0000+000</td>
<td>9.0000+000</td>
<td>9.0000+000</td>
<td>9.0000+000</td>
</tr>
<tr>
<td>J= 22</td>
<td>8.0000+000</td>
<td>8.0000+000</td>
<td>8.0000+000</td>
<td>8.0000+000</td>
<td>8.0000+000</td>
<td>8.0000+000</td>
<td>8.0000+000</td>
</tr>
<tr>
<td>J= 23</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
</tr>
<tr>
<td>J= 24</td>
<td>6.0000+000</td>
<td>6.0000+000</td>
<td>6.0000+000</td>
<td>6.0000+000</td>
<td>6.0000+000</td>
<td>6.0000+000</td>
<td>6.0000+000</td>
</tr>
<tr>
<td>I</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>----</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td></td>
</tr>
<tr>
<td>J=</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td>0.000+000</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>0.000+000</td>
<td>3.6140-002</td>
<td>4.6659-002</td>
<td>6.4327-002</td>
<td>1.1918-001</td>
<td>2.1412-001</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>0.000+000</td>
<td>4.7918-002</td>
<td>5.5637-002</td>
<td>6.8988-002</td>
<td>1.0754-001</td>
<td>1.6758-001</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.000+000</td>
<td>5.7113-002</td>
<td>6.1744-002</td>
<td>7.1436-002</td>
<td>7.3262-002</td>
<td>1.819-002</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>0.000+000</td>
<td>7.0004-002</td>
<td>6.9155-002</td>
<td>7.3262-002</td>
<td>9.1819-002</td>
<td>1.2199-001</td>
<td></td>
</tr>
</tbody>
</table>

K = 1

DISSIPATION RATE
<table>
<thead>
<tr>
<th>J</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>0.0000+000</td>
<td>8.3145-002</td>
<td>7.6718-002</td>
<td>7.6118-002</td>
<td>8.9667-002</td>
<td>1.1378-001</td>
<td>18</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>0.0000+000</td>
<td>9.8203-002</td>
<td>8.5256-002</td>
<td>7.9621-002</td>
<td>8.8659-002</td>
<td>1.0757-001</td>
<td>17</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0.0000+000</td>
<td>1.4913-001</td>
<td>1.1043-001</td>
<td>8.6294-002</td>
<td>8.2406-002</td>
<td>9.0976-002</td>
<td>16</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>0.0000+000</td>
<td>1.9777-001</td>
<td>1.3503-001</td>
<td>9.2176-002</td>
<td>7.5719-002</td>
<td>7.3934-002</td>
<td>15</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>0.0000+000</td>
<td>2.0985-001</td>
<td>1.4323-001</td>
<td>9.4064-002</td>
<td>7.0809-002</td>
<td>6.0258-002</td>
<td>14</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>0.0000+000</td>
<td>1.8318-001</td>
<td>1.3117-001</td>
<td>8.9145-002</td>
<td>6.6412-002</td>
<td>5.0699-002</td>
<td>13</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>0.0000+000</td>
<td>1.7447-001</td>
<td>1.2782-001</td>
<td>9.0212-002</td>
<td>6.9161-002</td>
<td>5.4751-002</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.0000+000</td>
<td>1.4951-001</td>
<td>1.1358-001</td>
<td>8.2669-002</td>
<td>6.4321-002</td>
<td>4.8670-002</td>
<td>11</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.0000+000</td>
<td>1.1911-001</td>
<td>9.4566-002</td>
<td>7.2367-002</td>
<td>5.8073-002</td>
<td>4.3563-002</td>
<td>10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.0000+000</td>
<td>1.0518-001</td>
<td>8.5210-002</td>
<td>6.6946-002</td>
<td>5.3656-002</td>
<td>3.9568-002</td>
<td>9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.0000+000</td>
<td>1.0085-001</td>
<td>8.2314-002</td>
<td>6.5225-002</td>
<td>5.3656-002</td>
<td>4.1243-002</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.0000+000</td>
<td>9.5451-002</td>
<td>7.8612-002</td>
<td>6.3004-002</td>
<td>5.2230-002</td>
<td>3.8120-002</td>
<td>7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.0000+000</td>
<td>7.3466-002</td>
<td>6.3321-002</td>
<td>5.3367-002</td>
<td>4.5836-002</td>
<td>3.6180-002</td>
<td>6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.0000+000</td>
<td>4.9501-002</td>
<td>4.5078-002</td>
<td>4.0468-002</td>
<td>3.6465-002</td>
<td>2.8670-002</td>
<td>5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.0000+000</td>
<td>3.3464-002</td>
<td>3.1842-002</td>
<td>3.0061-002</td>
<td>2.8300-002</td>
<td>2.1085-002</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.0000+000</td>
<td>2.3446-002</td>
<td>2.2989-002</td>
<td>2.2465-002</td>
<td>2.1919-002</td>
<td>1.3264-002</td>
<td>3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>1.7311-002</td>
<td>1.7281-002</td>
<td>1.7345-002</td>
<td>1.7651-002</td>
<td>1.7651-002</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>1.7308-002</td>
<td>1.7278-002</td>
<td>1.7258-002</td>
<td>1.7345-002</td>
<td>1.7651-002</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I=</td>
<td>19</td>
<td>20</td>
<td>21</td>
<td>22</td>
<td>23</td>
<td>24</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J=</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>8.9606-001</td>
<td>1.0688+000</td>
<td>1.3892+000</td>
<td>1.2279+000</td>
<td>8.2554-001</td>
<td>4.918-001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>8.4046-001</td>
<td>8.5893+000</td>
<td>9.4669+000</td>
<td>8.0201-001</td>
<td>5.4270-001</td>
<td>3.0970-001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>8.6901-001</td>
<td>7.2588+000</td>
<td>6.5109+000</td>
<td>5.3111+000</td>
<td>3.7459-001</td>
<td>2.836-001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>1.1254+000</td>
<td>7.3247-001</td>
<td>5.1282-001</td>
<td>3.8757-001</td>
<td>2.7836-001</td>
<td>1.8460-001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>1.5837+000</td>
<td>8.4463-001</td>
<td>4.9185-001</td>
<td>3.4475-001</td>
<td>2.4527-001</td>
<td>1.6610-001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>2.0976+000</td>
<td>9.7727-001</td>
<td>4.9110-001</td>
<td>3.1888-001</td>
<td>2.2284-001</td>
<td>1.5254-001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>3.3682+000</td>
<td>1.1237+000</td>
<td>4.7011-001</td>
<td>2.6783-001</td>
<td>1.7767-001</td>
<td>1.2240-001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>6.8140+000</td>
<td>1.4011+000</td>
<td>3.9058-001</td>
<td>2.0141-001</td>
<td>1.3456-001</td>
<td>9.4912-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>1.2611+000</td>
<td>1.5451+000</td>
<td>2.1949-001</td>
<td>1.3177-001</td>
<td>9.7521-002</td>
<td>7.2273-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>2.1723+000</td>
<td>1.5261+000</td>
<td>1.1074-001</td>
<td>8.7013-002</td>
<td>7.0949-002</td>
<td>5.4828-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>3.0503+000</td>
<td>1.1499+000</td>
<td>7.7067-002</td>
<td>7.2807-002</td>
<td>6.3702-002</td>
<td>5.0558-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>2.5514+000</td>
<td>6.9159-001</td>
<td>6.1661-002</td>
<td>5.7293-002</td>
<td>5.1405-002</td>
<td>4.2571-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>1.3219+000</td>
<td>5.2587-001</td>
<td>6.0450-002</td>
<td>5.4919-002</td>
<td>4.9754-002</td>
<td>4.1834-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>1.0885+000</td>
<td>4.5319-001</td>
<td>5.9528-002</td>
<td>5.3767-002</td>
<td>4.8788-002</td>
<td>4.1255-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>8.4929+000</td>
<td>3.7854-001</td>
<td>5.8381-002</td>
<td>5.2361-002</td>
<td>4.7656-002</td>
<td>4.0618-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1.4035+000</td>
<td>1.4772-001</td>
<td>5.1216-002</td>
<td>4.5647-002</td>
<td>4.2069-002</td>
<td>3.8375-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>5.4660-001</td>
<td>1.2569-001</td>
<td>6.4199-002</td>
<td>5.8653-002</td>
<td>5.4558-002</td>
<td>5.0661-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2.1028-001</td>
<td>1.6530-001</td>
<td>1.4545-001</td>
<td>1.3563-001</td>
<td>1.2524-001</td>
<td>1.1624-001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I=</td>
<td>25</td>
<td>26</td>
<td>27</td>
<td>28</td>
<td>29</td>
<td>30</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J=</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>1.8866-001</td>
<td>1.0655+000</td>
<td>5.5178-002</td>
<td>3.7941-002</td>
<td>2.6361-002</td>
<td>2.6388-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>1.0449-001</td>
<td>8.0140-002</td>
<td>6.2734-002</td>
<td>5.5080-002</td>
<td>5.0150-002</td>
<td>5.0158-002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I=</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td>------</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J=</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>3.8478-006</td>
<td>3.4047-005</td>
<td>3.0051-005</td>
<td>2.8989-005</td>
<td>3.4632-005</td>
<td>4.9385-005</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>3.8478-006</td>
<td>2.7142-004</td>
<td>2.5045-004</td>
<td>2.3260-004</td>
<td>2.3272-004</td>
<td>2.7199-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>3.8478-006</td>
<td>5.5019-004</td>
<td>5.3040-004</td>
<td>4.9911-004</td>
<td>4.6968-004</td>
<td>4.8738-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>3.8478-006</td>
<td>5.8768-004</td>
<td>5.7204-004</td>
<td>5.4162-004</td>
<td>5.0776-004</td>
<td>5.1733-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>3.8478-006</td>
<td>6.1419-004</td>
<td>6.0230-004</td>
<td>5.7468-004</td>
<td>5.3896-004</td>
<td>5.4162-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>3.8478-006</td>
<td>7.1505-004</td>
<td>7.0892-004</td>
<td>7.2326-004</td>
<td>7.2127-004</td>
<td>6.8126-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>3.8478-006</td>
<td>7.1640-004</td>
<td>7.2168-004</td>
<td>7.5137-004</td>
<td>7.8073-004</td>
<td>8.1170-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>3.8478-006</td>
<td>7.3188-004</td>
<td>7.4008-004</td>
<td>7.7235-004</td>
<td>8.0780-004</td>
<td>8.6459-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>3.8478-006</td>
<td>7.9321-004</td>
<td>8.1243-004</td>
<td>8.5463-004</td>
<td>9.0300-004</td>
<td>1.0039-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>3.8478-006</td>
<td>8.0402-004</td>
<td>8.2410-004</td>
<td>8.6680-004</td>
<td>9.1591-004</td>
<td>1.0194-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>3.8478-006</td>
<td>8.1775-004</td>
<td>8.3910-004</td>
<td>8.8238-004</td>
<td>9.3231-004</td>
<td>1.0387-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>3.8478-006</td>
<td>1.0684-003</td>
<td>1.0893-003</td>
<td>1.1267-003</td>
<td>1.1739-003</td>
<td>1.2839-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>3.8478-006</td>
<td>1.2922-003</td>
<td>1.3139-003</td>
<td>1.3437-003</td>
<td>1.3838-003</td>
<td>1.4747-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>3.8478-006</td>
<td>1.5536-003</td>
<td>1.5691-003</td>
<td>1.5890-003</td>
<td>1.6167-003</td>
<td>1.6752-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>3.8478-006</td>
<td>1.7989-003</td>
<td>1.8064-003</td>
<td>1.8153-003</td>
<td>1.8261-003</td>
<td>1.8449-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>3.8478-006</td>
<td>1.7990-003</td>
<td>1.8066-003</td>
<td>1.8155-003</td>
<td>1.8262-003</td>
<td>1.8450-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

I= 7, 8, 9, 10, 11, 12

J= 23, 22, 21, 20, 19, 18, 17
<table>
<thead>
<tr>
<th></th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0511-003</td>
<td>1.0567-003</td>
<td>1.0699-003</td>
<td>1.0960-003</td>
<td>8.5399-004</td>
<td>1.4918-003</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td>2</td>
<td>1.0700-003</td>
<td>1.0777-003</td>
<td>1.0924-003</td>
<td>1.1171-003</td>
<td>8.6381-004</td>
<td>1.3792-003</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>1.0939-003</td>
<td>1.1049-003</td>
<td>1.1220-003</td>
<td>1.1448-003</td>
<td>8.7717-004</td>
<td>1.2550-003</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>5</td>
<td>1.3742-003</td>
<td>1.4196-003</td>
<td>1.4503-003</td>
<td>1.4266-003</td>
<td>1.0415-003</td>
<td>9.2989-004</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>6</td>
<td>1.5585-003</td>
<td>1.6027-003</td>
<td>1.6202-003</td>
<td>1.5473-003</td>
<td>1.1478-003</td>
<td>1.0148-003</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>7</td>
<td>1.7286-003</td>
<td>1.7498-003</td>
<td>1.7385-003</td>
<td>1.6203-003</td>
<td>1.2394-003</td>
<td>1.1057-003</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>8</td>
<td>1.8518-003</td>
<td>1.8370-003</td>
<td>1.7917-003</td>
<td>1.6423-003</td>
<td>1.3301-003</td>
<td>1.2424-003</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>9</td>
<td>1.8519-003</td>
<td>1.8370-003</td>
<td>1.7917-003</td>
<td>1.6423-003</td>
<td>1.3301-003</td>
<td>1.2424-003</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0511-003</td>
<td>1.0567-003</td>
<td>1.0699-003</td>
<td>1.0960-003</td>
<td>8.5399-004</td>
<td>1.4918-003</td>
<td>9</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1.0700-003</td>
<td>1.0777-003</td>
<td>1.0924-003</td>
<td>1.1171-003</td>
<td>8.6381-004</td>
<td>1.3792-003</td>
<td>8</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1.0939-003</td>
<td>1.1049-003</td>
<td>1.1220-003</td>
<td>1.1448-003</td>
<td>8.7717-004</td>
<td>1.2550-003</td>
<td>7</td>
<td>7</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1.3742-003</td>
<td>1.4196-003</td>
<td>1.4503-003</td>
<td>1.4266-003</td>
<td>1.0415-003</td>
<td>9.2989-004</td>
<td>5</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1.5585-003</td>
<td>1.6027-003</td>
<td>1.6202-003</td>
<td>1.5473-003</td>
<td>1.1478-003</td>
<td>1.0148-003</td>
<td>4</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>1.7286-003</td>
<td>1.7498-003</td>
<td>1.7385-003</td>
<td>1.6203-003</td>
<td>1.2394-003</td>
<td>1.1057-003</td>
<td>3</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>1.8518-003</td>
<td>1.8370-003</td>
<td>1.7917-003</td>
<td>1.6423-003</td>
<td>1.3301-003</td>
<td>1.2424-003</td>
<td>2</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>1.8519-003</td>
<td>1.8370-003</td>
<td>1.7917-003</td>
<td>1.6423-003</td>
<td>1.3301-003</td>
<td>1.2424-003</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0511-003</td>
<td>1.0567-003</td>
<td>1.0699-003</td>
<td>1.0960-003</td>
<td>8.5399-004</td>
<td>1.4918-003</td>
<td>9</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1.0700-003</td>
<td>1.0777-003</td>
<td>1.0924-003</td>
<td>1.1171-003</td>
<td>8.6381-004</td>
<td>1.3792-003</td>
<td>8</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1.0939-003</td>
<td>1.1049-003</td>
<td>1.1220-003</td>
<td>1.1448-003</td>
<td>8.7717-004</td>
<td>1.2550-003</td>
<td>7</td>
<td>7</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1.3742-003</td>
<td>1.4196-003</td>
<td>1.4503-003</td>
<td>1.4266-003</td>
<td>1.0415-003</td>
<td>9.2989-004</td>
<td>5</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1.5585-003</td>
<td>1.6027-003</td>
<td>1.6202-003</td>
<td>1.5473-003</td>
<td>1.1478-003</td>
<td>1.0148-003</td>
<td>4</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>1.7286-003</td>
<td>1.7498-003</td>
<td>1.7385-003</td>
<td>1.6203-003</td>
<td>1.2394-003</td>
<td>1.1057-003</td>
<td>3</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>1.8518-003</td>
<td>1.8370-003</td>
<td>1.7917-003</td>
<td>1.6423-003</td>
<td>1.3301-003</td>
<td>1.2424-003</td>
<td>2</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>1.8519-003</td>
<td>1.8370-003</td>
<td>1.7917-003</td>
<td>1.6423-003</td>
<td>1.3301-003</td>
<td>1.2424-003</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>J=</td>
<td>23</td>
<td>22</td>
<td>21</td>
<td>20</td>
<td>19</td>
<td>18</td>
<td>17</td>
<td>16</td>
<td>15</td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>I=</td>
<td>25</td>
<td>26</td>
<td>27</td>
<td>28</td>
<td>29</td>
<td>30</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>5.6974-004</td>
<td>5.6993-004</td>
<td>5.7012-004</td>
<td>5.7023-004</td>
<td>5.7034-004</td>
<td>5.7045-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>5.6974-004</td>
<td>5.7012-004</td>
<td>5.7034-004</td>
<td>5.7056-004</td>
<td>5.7068-004</td>
<td>5.7080-004</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

K = 1  KINEM TURB VISC

<table>
<thead>
<tr>
<th>J=</th>
<th>23</th>
<th>22</th>
<th>21</th>
<th>20</th>
<th>19</th>
<th>18</th>
<th>17</th>
<th>16</th>
<th>15</th>
<th>14</th>
<th>13</th>
</tr>
</thead>
<tbody>
<tr>
<td>I=</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>1.1130-003</td>
<td>4.7026-004</td>
<td>5.6393-004</td>
<td>6.3699-004</td>
<td>6.6763-004</td>
<td>6.5399-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>1.2049-003</td>
<td>4.6681-004</td>
<td>5.5706-004</td>
<td>6.2283-004</td>
<td>6.5511-004</td>
<td>6.5399-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>1.2249-003</td>
<td>4.6430-004</td>
<td>7.1418-004</td>
<td>7.1343-004</td>
<td>7.3510-004</td>
<td>7.4100-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1.3066-003</td>
<td>5.5706-004</td>
<td>8.5403-004</td>
<td>8.3877-004</td>
<td>8.5396-004</td>
<td>8.6496-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>7.3330-004</td>
<td>7.3882-004</td>
<td>1.0388-003</td>
<td>1.0533-003</td>
<td>1.0632-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>7.3330-004</td>
<td>7.3882-004</td>
<td>1.0388-003</td>
<td>1.0533-003</td>
<td>1.0632-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>3.1366-004</td>
<td>2.7457-004</td>
<td>3.0622-004</td>
<td>3.1218-004</td>
<td>3.0575-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.0000+000</td>
<td>9.9155-004</td>
<td>1.0103-003</td>
<td>1.0594-003</td>
<td>1.1161-003</td>
<td>1.2322-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.0000+000</td>
<td>9.9465-004</td>
<td>9.5711-004</td>
<td>9.9905-004</td>
<td>1.0451-003</td>
<td>1.1190-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.0000+000</td>
<td>9.2632-004</td>
<td>9.3318-004</td>
<td>9.7178-004</td>
<td>1.0099-003</td>
<td>1.0502-003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.0000+000</td>
<td>9.2456-004</td>
<td>9.1659-004</td>
<td>9.3523-004</td>
<td>9.3265-004</td>
<td>8.8064-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.0000+000</td>
<td>9.0807-004</td>
<td>8.9979-004</td>
<td>9.0374-004</td>
<td>8.7282-004</td>
<td>8.1682-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.0000+000</td>
<td>8.5371-004</td>
<td>8.4782-004</td>
<td>8.3202-004</td>
<td>8.302-004</td>
<td>7.8732-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.0000+000</td>
<td>7.9344-004</td>
<td>7.7799-004</td>
<td>7.4208-004</td>
<td>6.9564-004</td>
<td>6.9911-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>1.1925-004</td>
<td>2.0062-004</td>
<td>3.0955-004</td>
<td>4.4681-004</td>
<td>5.9590-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>1.0402-004</td>
<td>1.0663-004</td>
<td>1.1218-004</td>
<td>1.1857-004</td>
<td>1.3202-004</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**I=*/  |    |    |    |    |    |    |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>0.0000+000</td>
<td>9.155-004</td>
<td>1.0103-003</td>
<td>1.0594-003</td>
<td>1.1161-003</td>
<td>1.2322-003</td>
</tr>
<tr>
<td>12</td>
<td>0.0000+000</td>
<td>9.4645-004</td>
<td>9.5711-004</td>
<td>9.9905-004</td>
<td>1.0451-003</td>
<td>1.1190-003</td>
</tr>
<tr>
<td>11</td>
<td>0.0000+000</td>
<td>9.2632-004</td>
<td>9.3318-004</td>
<td>9.7178-004</td>
<td>1.0099-003</td>
<td>1.0502-003</td>
</tr>
<tr>
<td>9</td>
<td>0.0000+000</td>
<td>9.2456-004</td>
<td>9.1659-004</td>
<td>9.3523-004</td>
<td>9.3265-004</td>
<td>8.8064-004</td>
</tr>
<tr>
<td>8</td>
<td>0.0000+000</td>
<td>9.0807-004</td>
<td>8.9979-004</td>
<td>9.0374-004</td>
<td>8.7282-004</td>
<td>8.1682-004</td>
</tr>
<tr>
<td>7</td>
<td>0.0000+000</td>
<td>8.5371-004</td>
<td>8.4782-004</td>
<td>8.3202-004</td>
<td>8.302-004</td>
<td>7.8732-004</td>
</tr>
<tr>
<td>6</td>
<td>0.0000+000</td>
<td>7.9344-004</td>
<td>7.7799-004</td>
<td>7.4208-004</td>
<td>6.9564-004</td>
<td>6.9911-004</td>
</tr>
<tr>
<td>5</td>
<td>0.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
</tr>
<tr>
<td>4</td>
<td>0.0000+000</td>
<td>1.1925-004</td>
<td>2.0062-004</td>
<td>3.0955-004</td>
<td>4.4681-004</td>
<td>5.9590-004</td>
</tr>
<tr>
<td>3</td>
<td>0.0000+000</td>
<td>1.0402-004</td>
<td>1.0663-004</td>
<td>1.1218-004</td>
<td>1.1857-004</td>
<td>1.3202-004</td>
</tr>
</tbody>
</table>

**J=*/  |    |    |    |    |    |    |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>6</td>
<td>0.0000+000</td>
<td>1.6748-003</td>
<td>1.7030-003</td>
<td>1.7418-003</td>
<td>1.7939-003</td>
<td>1.9121-003</td>
</tr>
<tr>
<td>5</td>
<td>0.0000+000</td>
<td>1.3793-003</td>
<td>1.4111-003</td>
<td>1.4598-003</td>
<td>1.5210-003</td>
<td>1.6640-003</td>
</tr>
<tr>
<td>4</td>
<td>0.0000+000</td>
<td>1.0502+000</td>
<td>1.0663+000</td>
<td>1.1218+000</td>
<td>1.1857+000</td>
<td>1.3202+000</td>
</tr>
<tr>
<td>3</td>
<td>0.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
<td>7.0000+000</td>
</tr>
<tr>
<td>2</td>
<td>0.0000+000</td>
<td>2.3335-003</td>
<td>2.3433-003</td>
<td>2.3549-003</td>
<td>2.3689-003</td>
<td>2.3933-003</td>
</tr>
<tr>
<td>1</td>
<td>0.0000+000</td>
<td>2.3337-003</td>
<td>2.3435-003</td>
<td>2.3552-003</td>
<td>2.3691-003</td>
<td>2.3934-003</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>15</td>
<td>16</td>
<td>17</td>
<td>18</td>
<td>19</td>
</tr>
<tr>
<td>---</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
<td>----</td>
</tr>
<tr>
<td>14</td>
<td>1.6089-003</td>
<td>1.7849-003</td>
<td>1.8260-003</td>
<td>1.7923-003</td>
<td>1.6742-003</td>
<td>1.4468-003</td>
</tr>
<tr>
<td>15</td>
<td>1.8461-003</td>
<td>2.0982-003</td>
<td>2.1657-003</td>
<td>2.1230-003</td>
<td>1.9576-003</td>
<td>1.6481-003</td>
</tr>
<tr>
<td>16</td>
<td>2.0756-003</td>
<td>2.4437-003</td>
<td>2.5637-003</td>
<td>2.5195-003</td>
<td>2.2890-003</td>
<td>1.8344-003</td>
</tr>
<tr>
<td>17</td>
<td>2.1424-003</td>
<td>2.5293-003</td>
<td>2.6449-003</td>
<td>2.5960-003</td>
<td>2.3496-003</td>
<td>1.8709-003</td>
</tr>
<tr>
<td>18</td>
<td>2.4377-003</td>
<td>2.8988-003</td>
<td>3.0555-003</td>
<td>3.0253-003</td>
<td>2.7607-003</td>
<td>2.1419-003</td>
</tr>
<tr>
<td>20</td>
<td>2.7271-003</td>
<td>2.9229-003</td>
<td>3.0442-003</td>
<td>3.0621-003</td>
<td>2.9551-003</td>
<td>2.8233-003</td>
</tr>
<tr>
<td>21</td>
<td>2.0835-003</td>
<td>2.4868-003</td>
<td>2.5516-003</td>
<td>2.5584-003</td>
<td>2.4971-003</td>
<td>2.0910-003</td>
</tr>
<tr>
<td>22</td>
<td>1.7047-003</td>
<td>9.8091-004</td>
<td>8.4601-004</td>
<td>8.4973-004</td>
<td>8.0210-003</td>
<td>1.6569-003</td>
</tr>
<tr>
<td>23</td>
<td>1.5901-003</td>
<td>6.3029-004</td>
<td>4.6656-004</td>
<td>4.6013-004</td>
<td>6.3563-004</td>
<td>1.4564-003</td>
</tr>
<tr>
<td>24</td>
<td>1.5479-003</td>
<td>5.1566-004</td>
<td>3.1972-004</td>
<td>2.9408-004</td>
<td>4.5248-004</td>
<td>1.2491-003</td>
</tr>
<tr>
<td>26</td>
<td>2.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>27</td>
<td>1.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>28</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>29</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>30</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>---</td>
<td>-----</td>
<td>------------</td>
<td>------------</td>
<td>------------</td>
<td>------------</td>
<td>------------</td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>1.1228-003</td>
<td>1.1284-003</td>
<td>1.1299-003</td>
<td>1.1329-003</td>
<td>1.1339-003</td>
</tr>
<tr>
<td>9</td>
<td></td>
<td>1.2138-003</td>
<td>1.2210-003</td>
<td>1.2229-003</td>
<td>1.2261-003</td>
<td>1.2273-003</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td>1.2391-003</td>
<td>1.2466-003</td>
<td>1.2487-003</td>
<td>1.2519-003</td>
<td>1.2531-003</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>1.2693-003</td>
<td>1.2771-003</td>
<td>1.2791-003</td>
<td>1.2824-003</td>
<td>1.2836-003</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>1.3819-003</td>
<td>1.3867-003</td>
<td>1.3882-003</td>
<td>1.3910-003</td>
<td>1.3922-003</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>1.4263-003</td>
<td>1.4262-003</td>
<td>1.4261-003</td>
<td>1.4276-003</td>
<td>1.4282-003</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>1.2693-003</td>
<td>1.2695-003</td>
<td>1.2687-003</td>
<td>1.2693-003</td>
<td>1.2694-003</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
<td>0.0000+000</td>
</tr>
</tbody>
</table>
Sheng-Yang Ju was born on October 20, 1958 in Taipei, Taiwan. He lived with his family in Taipei, and graduated from National Taiwan University with a Bachelor of Science Degree in Chemical Engineering in June 1980. After having served two-year military service, he enrolled at Louisiana State University in August 1982. He married Ms. Tung-Ning Chang at Baton Rouge in December 1982. In May 1984, he had a boy and received a Master of Science Degree in Chemical Engineering. In August 1985, he had his second son. He is a candidate for a Philosophy of Science Degree in Chemical Engineering in August 1987.
DOCTORAL EXAMINATION AND DISSERTATION REPORT

Candidate: Sheng-Yang Ju

Major Field: Chemical Engineering

Title of Dissertation: Three-Dimensional Turbulent Flowfield in a Turbine Stirred Tank

Approved:

[Signatures]

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

DATE OF EXAMINATION:

July 16, 1987