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A NUMERICAL INVESTIGATION OF TURBULENT INTERCHANGE
MIXING OF AXIAL COOLANT FLOW IN ROD BUNDLE GEOMETRIES

by

Ross C. K. Rock

A thesis submitted in conformity with the requirements
for the degree of Master of Applied Science
Graduate Department of Mechanical and Industrial Engineering
University of Toronto

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Abstract

A Numerical Investigation of Turbulent Interchange Mixing of Axial Coolant Flow in Rod Bundle Geometries

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1998

Turbulent coolant flow mixing within an array of nuclear fuel rods is an essential mechanism for maintaining a uniform distribution of heat throughout the array. Of the various coolant mixing mechanisms, turbulent interchange mixing is one of the more important. Using a three dimensional numerical solution, the characteristics and appropriateness of an isotropic $k - \varepsilon$ turbulence model for use in modeling turbulent interchange mixing within rod arrays was investigated. The isotropic model accurately predicted the radial component of turbulent eddy viscosity, but underpredicted the azimuthal component. As a result, radial diffusion processes (such as pressure drop) were predicted accurately, but azimuthal diffusion processes (such as turbulent interchange mixing) were underpredicted. An isotropic eddy viscosity turbulence model, therefore, is not recommended for analysis of turbulent interchange mixing.

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Contents

List of Tables	ix
List of Figures	xi
Nomenclature	xiv
1 Introduction	1
1.1 Background	1
1.2 Relevance of Research to Nuclear Safety Analysis	3
1.3 Objectives and Scope	3
1.4 Structure of Thesis Document	4
2 Literature Review	5
2.1 Overview	5
2.2 Behaviour of Coolant Flow in Rod Bundles	5
2.2.1 Law of the Wall	5
2.2.2 Transition to Turbulence	8
2.2.3 Turbulent Friction Factor for Fully Developed Flow	9
2.2.4 Turbulent Velocity Fluctuations	11
2.2.5 Wall Shear Distribution	13
2.2.6 Turbulent Eddy Diffusivity Anisotropy	15
2.3 Coolant Mixing Mechanisms	18
2.4 Subchannel Models of Coolant Mixing by Turbulent Interchange	19
2.4.1 Subchannel Approach to Modeling	19
2.4.2 Subchannel Models of Turbulent Interchange Mixing	20
2.4.3 Additional Mixing Models	22
2.4.4 Comparison of Mixing Models	23
2.4.5 Dependence of Mixing on Pitch-to-Diameter Ratio, γ_p	26

2.5	Contribution of Secondary Flow to Mixing	27
2.6	Turbulent Prandtl Number	29
2.7	Influence of Friction Factor on Mixing	30
2.8	Flow Pulsations in Gap	30
2.9	Limitations of Integrated Models of Turbulent Interchange Mixing	32
2.10	Summary	33
3	Mathematical Model and Numerical Solution	35
3.1	Mathematical Model	35
3.1.1	Instantaneous Quantities and Time Averaging	35
3.1.2	Conservation of Mass	36
3.1.3	Conservation of Momentum	37
3.1.4	Buoyancy Model	38
3.1.5	Eddy Viscosity Model of Turbulence	39
3.1.6	$k - \varepsilon$ Turbulence Model	41
3.1.7	Conservation of Energy	42
3.1.8	Boundary Conditions	43
	Wall Boundaries	43
	Inlet Boundaries	44
	Outlet Boundaries	45
	Symmetry Boundaries	45
3.2	Numerical Solution	46
3.2.1	Discretization of Domain	46
3.2.2	Discretization of Governing Equations	47
3.2.3	Three-Dimensional Representation	49
3.2.4	Discretization of Boundary Conditions	49
	Wall Boundary	50
	Inlet Boundary	51
	Outlet Boundary	51
	Symmetry Boundary	52
3.2.5	Grid Colocation	52
3.2.6	Solution of Equations	53
3.3	Summary	54
4	Preliminary Validation Studies	56
4.1	Overview	56

4.2	Laminar Flow in a Circular Pipe	57
4.2.1	Description of Problem and Analytical Solution	57
4.2.2	Boundary Conditions and Simulation Details	58
4.2.3	Analysis of Results	60
4.3	Laminar Heat Transfer in a Circular Pipe	62
4.3.1	Description of Problem and Analytical Solution	62
4.3.2	Boundary Conditions and Simulation Details	63
4.3.3	Analysis of Results	64
4.4	Turbulent Flow in a Circular Pipe	66
4.4.1	Description of Problem and Analytical Solution	66
4.4.2	Boundary Conditions and Simulation Details	67
4.4.3	Analysis of Results	68
4.5	Turbulent Heat Transfer in a Circular Pipe	72
4.5.1	Description of Problem and Analytical Solution	72
4.5.2	Boundary Conditions and Simulation Details	72
4.5.3	Analysis of Results	73
4.6	Laminar Buoyancy-Driven Convection in a Square Cavity	74
4.6.1	Description of Problem and Benchmark Solution	74
4.6.2	Boundary Conditions and Simulation Details	76
4.6.3	Analysis of Results	77
4.7	Summary of Preliminary Validation	81
5	Final Validation Studies	83
5.1	Selection of Validation Dataset	83
5.2	Final Validation Study Dataset	84
5.2.1	Description of Experiment	84
5.2.2	Solution Domain and Boundary Conditions	86
5.2.3	Solution Methodology	90
	Mechanical Flow Solution	90
	Thermal Solution	91
5.3	Validation Study Results	92
5.3.1	Axial Velocity Distribution	92
5.3.2	Effective Turbulent Thermal Conductivity, Γ_{eff}	95
5.3.3	Temperature Fields	98
5.3.4	Wall Shear	102
5.4	Summary	104

6	Analysis of Validation Results	106
6.1	Overview	106
6.2	Predicted Friction Factor	106
6.3	Turbulent Interchange Mixing	109
6.4	Dependence of Mixing and Friction on Reynolds Number	114
6.5	Distribution of Turbulent Eddy Diffusivity in the Gap	116
6.6	Discussion of Isotropic Turbulent Eddy Diffusivity Model	119
6.7	Mesh Sensitivity Studies	121
6.7.1	Mesh Resolution and Near-Wall Node Position Sensitivity	122
6.7.2	Inlet Turbulence Parameter Sensitivity	126
6.8	Summary	127
7	Closure	129
7.1	Summary and Conclusions	129
7.2	Recommendations for Further Work	130
	Bibliography	130
	Appendices	138
A	Secondary Flows	138
B	Evaluation of Diffusion and Advection Terms	141
B.1	Evaluation of Diffusion Term	141
B.2	Evaluation of Advection Term	142
C	The Colocated Grid	146
C.1	Pressure / Velocity Coupling and Grid Colocation	146
C.2	Transient Multidimensional Representation	150
C.3	Order of Convergence and Stability	152
D	Convergence Behaviour of Point Solvers	153
E	Multigrid	156
F	Table of Experimental Datasets	159
G	Seale Experiment Mesh Generation Using TASCgrid	163
G.1	Geometry Definition	164

G.1.1	Key Points	164
G.1.2	global_parameters File	165
G.1.3	GDF File	166
G.2	Curve Definition	169
G.2.1	Key Points	169
G.2.2	CDF File	171
G.3	Surface Definition	174
G.3.1	Key Points	174
G.3.2	SDF File	175
G.4	Internal Definition	175
G.4.1	Key Points	175
G.4.2	IDF File	175
H	Thermal Solution Modifications	176
H.1	TASCtool Macro write_cond	176
H.2	Subroutine propt.f Modifications	176
H.3	Subroutine userpp.f Modifications	182

List of Tables

2.1	Velocity Laws of the Wall	8
2.2	Temperature Laws of the Wall	8
2.3	Mixing Mechanisms Identified by Rogers and Rosehart	18
2.4	Models of Turbulent Interchange	23
3.1	$k - \varepsilon$ Model Constants	42
4.1	Phenomena Studied in Preliminary Validation	57
4.2	Boundary Conditions and Fluid Properties for Laminar Flow in a Circular Pipe	59
4.3	Length Required for Development of Laminar Flow	60
4.4	Analytical and Predicted Pressure Gradient for Laminar Flow in a Circular Pipe	61
4.5	Thermal Properties for Laminar Flow in Heated Pipe	64
4.6	Boundary Conditions and Fluid Properties for Turbulent Flow in a Circular Pipe	68
4.7	Turbulent Heat Transfer Ratio $(T_w - T_b)/(T_w - T_c)$	73
4.8	Turbulent Heat Transfer in a Circular Pipe Boundary Conditions	73
4.9	Predicted Turbulent Heat Transfer in Circular Pipe	74
4.10	Boundary Conditions for Buoyancy-Driven Flow in a Square Cavity	76
4.11	Results for Rayleigh Number of 10^3	78
4.12	Results for Rayleigh Number of 10^4	78
4.13	Results for Rayleigh Number of 10^5	78
4.14	Convergence and Extrapolation Results	79
5.1	Geometry Data for Seale's Apparatus	84
5.2	Measurement Uncertainties Reported by Seale	86
5.3	Mesh Geometric Properties	88
5.4	Fluid Properties for Final Validation Dataset	88

5.5	Summary of Final Validation Inlet Mass Flows	89
5.6	Measured and Predicted Gap Velocity Ratios	95
6.1	Results of Linear Regression of Friction Factor Results	109
6.2	Code Predicted Gap Stanton Numbers	110
6.3	Results of Linear Regression of Gap Stanton Number Results	113
6.4	Ratio of b_f to b_s	116
6.5	Mesh Resolution Sensitivity Parameters	122
6.6	Sensitivity to Inlet Turbulence Parameters	127
F.1	Table of Experimental Rod Bundle Datatsets	159
G.1	Point Variable Naming Convention	166
G.2	Wall Function Node Control Points	171

List of Figures

1.1	Schematic of Coolant Mixing in an Array of Rods	2
2.1	Fanning Friction Factor	10
2.2	Velocity Fluctuation Distribution in Rod-Wall Geometry	12
2.3	Distribution of Wall Shear on Rod Surface	14
2.4	Distribution of Wall Shear on Rod Surface (Rod/Wall Geometry)	15
2.5	Normalized Radial Eddy Viscosity in Rod-Wall Geometry	17
2.6	Square, Triangular and Wall Subchannels	19
2.7	Turbulent Interchange Models for Square Subchannels	26
2.8	Turbulent Interchange Models for Triangular Subchannels	27
2.9	Turbulent Interchange Models for Mixed Subchannel Geometries	28
3.1	Schematic of Two-Dimensional Control Volume	46
3.2	Two-Dimensional Finite Elements and Integration Points	48
3.3	Three Dimensional Control Volume Octant	50
4.1	Quarter Butterfly Grid used for Laminar Pipe Flow	58
4.2	Error in Prediction of Laminar Axial Velocity Profile $U(r)$	61
4.3	Nusselt Numbers for Laminar Flow in a Heated Pipe	65
4.4	Friction Factors for Turbulent Flow in a Pipe	69
4.5	Radial Profile of Turbulent Axial Velocity	70
4.6	Radial Profile of Axial Turbulent Intensity	71
4.7	Domain for Buoyancy Driven Flow in a Square Cavity	75
4.8	Natural Convection Temperature, θ , Contours	80
4.9	Natural Convection $\hat{U}$ Velocity Contours	80
4.10	Natural Convection $\hat{W}$ Velocity Contours	80
4.11	Logarithmic $\overline{Nu}$ Residual vs. Grid Size for Buoyancy-Driven Flow	81
5.1	Detail of 5 Rod Duct	85

5.2	Three Ducts used by Seale	85
5.3	Cross sections of meshes used for final validation	87
5.4	Axial Velocity Contours, $\gamma_p = 1.1$	93
5.5	Axial Velocity Contours, $\gamma_p = 1.375$	93
5.6	Axial Velocity Contours, $\gamma_p = 1.833$	94
5.7	Normalized Axial Velocity Contours, $\gamma_p = 1.375$, $Re=9.067 \times 10^4$	94
5.8	Normalized Turbulent Thermal Conductivity Contours, $\gamma_p = 1.1$	97
5.9	Normalized Turbulent Thermal Conductivity Contours, $\gamma_p = 1.375$	97
5.10	Normalized Turbulent Thermal Conductivity Contours, $\gamma_p = 1.833$	99
5.11	Normalized Temperature Contours, $\gamma_p = 1.1$	99
5.12	Normalized Temperature Contours, $\gamma_p = 1.375$	100
5.13	Normalized Temperature Contours, $\gamma_p = 1.833$	100
5.14	Normalized Temperature Contours, $\gamma_p = 1.375$	101
5.15	Normalized Wall Shear Around Rod, $\gamma_p = 1.1$	103
5.16	Normalized Wall Shear Around Rod, $\gamma_p = 1.375$	104
5.17	Normalized Wall Shear Around Rod, $\gamma_p = 1.833$	105
6.1	Predicted Friction Factors for Seale Experiment Duct 5, $\gamma_p = 1.1$	107
6.2	Predicted Friction Factors for Seale Experiment Duct 4, $\gamma_p = 1.375$	107
6.3	Predicted Friction Factors for Seale Experiment Duct 3, $\gamma_p = 1.833$	108
6.4	Predicted Gap Stanton Numbers for Seale Experiment, $\gamma_p = 1.1$	111
6.5	Predicted Gap Stanton Numbers for Seale Experiment, $\gamma_p = 1.375$	112
6.6	Predicted Gap Stanton Numbers for Seale Experiment, $\gamma_p = 1.833$	112
6.7	Comparison of code and experiment results with subchannel models	114
6.8	Predicted Normalized Eddy Viscosity, $\gamma_p = 1.1$	117
6.9	Predicted Normalized Eddy Viscosity, $\gamma_p = 1.375$	117
6.10	Predicted Normalized Eddy Viscosity, $\gamma_p = 1.833$	118
6.11	Friction Factor Sensitivity Study, $\gamma_p = 1.1$	123
6.12	Friction Factor Sensitivity Study, $\gamma_p = 1.375$	123
6.13	Friction Factor Sensitivity Study, $\gamma_p = 1.833$	124
6.14	Gap Stanton Number Sensitivity Study, $\gamma_p = 1.1$	125
6.15	Gap Stanton Number Sensitivity Study, $\gamma_p = 1.375$	125
6.16	Gap Stanton Number Sensitivity Study, $\gamma_p = 1.833$	126
B.1	One Dimensional Control Volume	143
B.2	Skewed upwinding in two dimensions	145

E.1	Multigrid ‘W-cycle’	158
G.1	Mesh Topology	164
G.2	Mesh Node Names	165
G.3	Mesh Layout	170

Nomenclature

<i>Symbol</i>	<i>Definition</i>
α	thermal diffusivity [m^2/s]
β	fluid thermal expansion coefficient [K^{-1}]
γ_p	pitch-to-diameter ratio (p/D)
Γ	molecular thermal conductivity [$W/m \cdot K$]
Γ_{eff}	effective thermal conductivity [$W/m \cdot K$] $= \Gamma + \Gamma_t$
Γ_t	turbulent thermal conductivity [$W/m \cdot K$] $= \mu_t c_p / Pr_t$
δ	distance between centroids of subchannels i and j [m]
ϵ_H	turbulent diffusivity of heat [m^2/s]
ϵ_M	turbulent diffusivity of momentum [m^2/s]
ϵ_M^r	turbulent diffusivity of momentum in the radial direction [m^2/s]
ϵ_M^φ	turbulent diffusivity of momentum in the azimuthal (circumferential) direction [m^2/s]
ε	turbulent dissipation rate [W/kg]
μ	molecular dynamic viscosity [$Pa \cdot s$]
μ_t	turbulent dynamic viscosity of momentum [$Pa \cdot s$] $= \rho \epsilon_M$
μ_t^+	normalized turbulent dynamic viscosity of momentum $= \mu_t / \rho \hat{r} U_\tau$
μ_t^H	turbulent dynamic viscosity of heat [$Pa \cdot s$] $= \rho \epsilon_H$
ν	molecular kinematic viscosity [m^2/s] $= \mu / \rho$
ρ	density [kg/m^3]

<i>Symbol</i>	<i>Definition</i>
τ_w	wall shear [Pa]
τ_{ij}^R	Reynolds stress tensor [Pa] $= \overline{u'_i u'_j}$
b	true gap width [m]
c_p	heat capacity at constant temperature [$J/kg \cdot K$]
c	effective gap width [m]
c_μ	eddy viscosity model proportionality constant
D	rod diameter [m]
D_h	hydraulic diameter [m]
f_p	characteristic frequency of gap flow pulsations [Hz]
g	gravitational acceleration ($9.81 [m/s^2]$)
Gr	Grashof number
Gz	Graetz number
h_i	enthalpy of subchannel i [$J/kg \cdot K$]
h_g	gap heat transfer coefficient [$W/m^2 \cdot K$]
h_w	wall heat transfer coefficient [$W/m^2 \cdot K$]
k	turbulent kinetic energy [J/kg]
k_w	wavenumber [m^{-1}]
M_{ij}	mass Stanton number between subchannels i and j
Nu	Nusselt number
N_n	shape function for node n
n	constant in Nikuradse's turbulent velocity profile eq'n
n_i	unit normal in i direction
$\overline{Nu}_L$	Length-averaged Nusselt number
P	pressure [Pa]
p	rod pitch (distance between centroids) [m]
Pr	Prandtl number
Pr_t	turbulent Prandtl number
Q	volumetric flow rate [m^3/s]
q'	net heat transport through gap per unit length [W/m]
q''_w	wall heat flux [W/m^2]
r	rod radius [m]
$\hat{r}$	distance from rod surface to symmetry line [m]

<i>Symbol</i>	<i>Definition</i>
Ra	Rayleigh number $= \text{GrPr}$
St_g	gap Stanton number $= q' / b \Delta T \rho U_b c_p$
St	Strouhal number $= f_p D / u_\tau$
T^+	dimensionless temperature
T_b	bulk temperature [K]
$\tilde{u}_i$	instantaneous velocity in i direction [m/s] $= \overline{U}_i + u'_i$
U_i	time-averaged or quasi-steady velocity in i direction [m/s]
u'_i	velocity fluctuations in i direction [m/s]
u'	axial velocity fluctuations [m/s]
U^+	dimensionless velocity near the wall $= U / U_\tau$ or $= c_\mu^{1/4} \sqrt{k}$
U_τ	shear velocity [m/s] $= \sqrt{\tau_w / \rho}$
U_b	axial bulk velocity [m/s]
U_g	axial velocity in the gap between rods [m/s]
U_t	velocity tangential to surface [m/s]
U_w	axial velocity in the gap between the rod and wall [m/s]
v'	velocity fluctuations in azimuthal direction [m/s]
w'	fictitious mass transfer attrib. to turb. mixing [kg/m · s]
x_i	distance in i direction [m]
y	distance from near-wall nodes to wall [m]
y^+	dimensionless distance from the wall $= \rho u_\tau y / \mu$
z_{ij}	effective temperature gradient distance [m]

Chapter 1

Introduction

1.1 Background

A characteristic of virtually all nuclear reactor designs is the use of long, cylindrical fuel rods comprised of ceramic uranium pellets clad in thin metallic sheathing. When arranged in bundles and moderated (*i.e.*, placed in a medium which *thermalizes* or ‘slows down’ emitted neutrons), the fuel rods undergo nuclear fission and produce heat. Large pumps force coolant axially through the fuel bundles thereby serving two purposes, one operational and one safety-related. The operational purpose of coolant is to transport fission heat from the fuel bundles to heat exchangers external to the reactor. These heat exchangers produce steam which is used to generate electricity. The safety-related purpose of coolant is to maintain the fuel rods and other reactor components at an acceptable operating temperature.

Understanding the physical behaviour of the coolant as it flows through the fuel bundles is of interest to those analysing reactor operation and safety. An important aspect of understanding this behaviour is the mixing of coolant momentum and heat. Without adequate coolant mixing models, the heat removal capabilities and safety margins of the reactor cannot be accurately established nor predicted. Figure 1.1 illustrates the direction of coolant mixing in an axially-dominated flow within an array of fuel rods.

Modeling of coolant mixing within bundles has been accomplished using a number of different approaches. Some models involve integration or ‘lumping’ of flow parameters into coarse control volumes called ‘subchannels’[1]. Mixing between subchannels is modeled by employing constitutive relations based upon a combination of theory and experimental observation. Such models tend to be very specific in their application; often they can only be used for the bundle geometry against which they were developed and

Figure 1.1: Schematic of Coolant Mixing in an Array of Rods

‘tuned.’ Further, the relatively coarse size of subchannels results in fewer control volumes in a given domain, thereby decreasing the computational effort required to solve a given problem.

Other approaches attempt to solve the fluid conservation equations on a scale smaller than that of subchannel models. Such ‘full-field’ solutions tend to be more general in their application since they are not developed for any particular geometry. Care must be taken, however, when using generalized models for specific applications. In particular, attention must be paid to the possibility of physical processes important to the specific application being absent or unresolvable by the full-field solution. In addition, the fine resolution of full-field solutions tend to increase the computational effort required to obtain a solution.

The most desirable approach to modeling coolant mixing would be one which provides the geometric flexibility of a ‘full-field’ solution with the computational efficiency of a well-designed subchannel model. An ideal solution methodology would provide the best combination of solution accuracy and computational cost. In order to develop such a methodology, an understanding of the physical and computational characteristics of both subchannel and full-field approaches is required.

1.2 Relevance of Research to Nuclear Safety Analysis

Coolant mixing influences the distribution of coolant enthalpy within the fuel bundles. A well-mixed coolant is essential to avoiding local ‘hot spots’ in the bundles. Hot spots can lead to the onset of nucleate boiling and patches of ‘dry-out’ (*i.e.* poor heat removal) on the fuel rod surfaces. Dry-out, in turn, leads to escalation of fuel and fuel cladding temperature. Hence, coolant mixing limits or eliminates undesireably high temperatures within the reactor. It is therefore desirable to determine how the coolant mixes within a fuel bundle as accurately as possible in order to predict the extent and consequences of local bundle hot spots. This requires robust models which can be relied upon to provide physically justifiable predictions.

This research will assist coolant mixing model development by providing a physical understanding of the mixing processes. Further, through investigation of the performance of a coolant mixing model, knowledge of the applicability range of such models will be improved. This will assist nuclear safety analysis by providing greater confidence in the physical correctness of predictions based on particular models of coolant mixing.

1.3 Objectives and Scope

The objective of this thesis is to use established physical, mathematical and numerical models to:

1. understand the physical behaviour of coolant mixing within a nuclear fuel bundle; and,
2. present a full-field coolant mixing model and assess its applicability to the study of coolant mixing within a nuclear fuel bundle.

A turbulent interchange mixing model will be presented to simulate steady, single phase axial coolant flow over a rod array. Turbulent interchange and its role in coolant mixing will be developed and explained as part of the literature review (Chapter 2).

As mentioned previously, one intent of this research is to identify the range of applicability of the turbulent interchange mixing model described in this thesis. Provided its applicability is demonstrated, the model can be used to address the correctness of other mixing models already in use by the nuclear safety analysis community.

The scope of this thesis is to use an existing computational fluid dynamics (CFD) code for simulating turbulent interchange mixing within an array of cylindrical rods.

The turbulence characteristics are modeled using a $k - \varepsilon$ model provided in the code. An explanation and discussion of the $k - \varepsilon$ turbulence model is provided in Chapter 3.

The code was developed as a general CFD package and was not specifically tailored to the application of coolant mixing in bundles. Hence, the ‘full-field’, as opposed to ‘subchannel’, approach will be used here. The applicability of a $k - \varepsilon$ model for use in investigating coolant mixing in rod bundles will be assessed through both review of the CFD code’s physical models and validation of code results against experiment.

1.4 Structure of Thesis Document

The objectives and scope discussed in the previous section will be met and demonstrated using the following structure.

1. In Chapter 2, a literature review will establish the depth and range of theoretical and experimental understanding of coolant mixing in rod bundles. Discussions pertaining to the roles of various physical phenomena related to coolant mixing will be provided. The physical processes of coolant mixing will be discussed with an emphasis on mixing by turbulent interchange. Subchannel-based turbulent interchange mixing models will be presented and discussed.
2. In Chapter 3, a model of mixing in rod bundles by turbulent interchange using the $k - \varepsilon$ turbulence model will be presented.
3. Preliminary validation of the CFD code and associated models will be presented in Chapter 4 through simulation of simple geometries and comparison against analytical and benchmark solutions.
4. An experiment which measured turbulent interchange mixing in an array of rods will be discussed in Chapter 5. Final validation of the model against the experiment’s results will be presented.
5. Analysis of the final validation results will be provided in Chapter 6. In particular, the performance of the model, based both on physical and numerical interpretation of the results, will be discussed.
6. Recommendations and conclusions pertaining to the use of the models discussed will be provided in Chapter 7.

Additional background material associated with the research will be provided in appendices.

Chapter 2

Literature Review

2.1 Overview

The first half of the literature review concentrates on the physical behaviour of coolant flow in rod bundles. This includes investigation of the near-wall behaviour of the flow, turbulent friction factors, velocity fluctuations, and wall shear distribution.

The second half of the literature review provides a discussion of coolant mixing, with an emphasis on mixing by turbulent interchange. After a description of the subchannel approach to modeling, different subchannel models of turbulent interchange mixing are presented and discussed.

The literature survey concludes with a summary and an identification of issues which require further research.

2.2 Behaviour of Coolant Flow in Rod Bundles

2.2.1 Law of the Wall

An important aspect of turbulent flows is the behaviour of the flow near a stationary wall. Very close to a wall, where viscous forces dominate over inertial, fluid turbulence cannot be sustained. As a result, there is no turbulence adjacent to the wall, and a viscous, or laminar, sub-layer is observed. Between the laminar sub-layer and the core of the flow there is a transition, or buffer layer and a region of logarithmic velocity increase. Properly accounting for the existence of these layers in turbulent flow is extremely important in predicting wall shear (and therefore pressure drop) accurately. The law of the wall models the relationship between axial flow velocity and wall distance in the logarithmic layer.

The distance from the wall, y , is non-dimensionalised using the local shear velocity, u_τ .

$$y^+ = \frac{\rho u_\tau y}{\mu} \quad (2.1)$$

where ρ and μ are the fluid density and dynamic viscosity, respectively. The local shear velocity, u_τ , is defined as follows.

$$u_\tau = \sqrt{\tau_w / \rho} \quad (2.2)$$

where τ_w is the local wall shear stress.

The non-dimensional velocity, u^+ , is the ratio of the local velocity, u , divided by the local shear velocity.

$$u^+ = \frac{u}{u_\tau} \quad (2.3)$$

Experimental measurements of pipe flow have found the boundaries between the three distinct flow regions (viscous, transition, and logarithmic) occur at specific values of y^+ [2]. The laminar sub-layer is observed for $y^+ < 5$, while the transition layer is observed in the range $5 < y^+ < 30$. For $y^+ > 30$ the relationship between u^+ and y^+ follows a logarithmic law.

$$u^+ = \frac{1}{\kappa} \ln y^+ + C_1 \quad (2.4)$$

where κ is the Von Karman constant, equal to 0.41, and C_1 is an empirical constant.

This logarithmic law of the wall is used as a boundary condition for many turbulence models, including the model presented later in this thesis. Modeling the viscous and transition layers, which are very thin, is often difficult and requires additional models. Using the law of the wall alone to capture the near-wall effects is often sufficient.

An upper limit on y^+ exists for the law of the wall to be applicable. This upper limit is often observed to be in the range of $y^+ = 100$ to 500, and is specific to flow conditions and geometry. Pipe flow typically exhibits an upper y^+ limit of approximately 300 [3].

The temperature law of the wall provides a similar relationship between dimensionless temperature and wall distance.

$$T^+ = \frac{1}{C_2} \ln y^+ + C_3 \quad (2.5)$$

C_2 and C_3 are empirical constants.

The dimensionless temperature, T^+ , is defined in terms of the wall heat flux, q_w'' , shear velocity, u_τ , and difference between the wall and free-stream fluid temperatures, $(T_w - T_f)$.

$$T^+ = \frac{\rho c_p u_\tau}{q_w''} (T_w - T_f) \quad (2.6)$$

Adiabatic walls are characterised by $q_w = 0$. The temperature law of the wall is not required in this circumstance.

While the law of the wall was developed for pipes, it is necessary to determine if a similar law holds for axial flow in rod bundles.

Krauss and Meyer [4] measured the dimensionless axial velocity profile in a geometry consisting of a rod placed near a wall. Starting at a dimensionless distance of approximately $y^+ = 90$ and extending out to $y^+ = 300$, it was found that the velocity profile followed the law of the wall quite closely. The slope of the profile in the rod-wall gap (*i.e.* $1/\kappa$) was slightly less than $1/0.40$, but matches $1/0.40$ very closely near the surface of the rod facing into the subchannel core and the gap between the rods.

The dimensionless temperature profiles, however, did not follow a similar trend. Using local friction velocities, the dimensionless temperature profile in the gap between rods was different from the profile between the rod and wall. The deviation was attributed to the “extremely asymmetric temperature distribution in the wall channel.”

Meyer [5] measured the velocity and temperature laws of the wall in a triangular subchannel (*i.e.* a subchannel between three rods). The velocity profile followed the law of the wall very closely from a y^+ value of 80 to approximately 600, with a small wake effect seen from $y^+ = 600$ to 1000. A wake effect is an increase in the additive constant in the law of the wall [3]. The velocity profile observed by Meyer was virtually the same regardless of radial position of the measurement with respect to the rod.

Hishida and Nagano [6] used a two-wire probe method of measuring fully developed turbulent flow in a circular pipe. They found heated and unheated flow exhibited slightly different law of the wall behaviour. While the unheated flow exhibited a form of $u^+ = 2.50 \ln y^+ + 5.5$, the heated flow exhibited a form of $u^+ = 2.50 \ln y^+ + 4.65$. Further, the temperature followed the form $T^+ = 2.17 \ln y^+ + 4.30$. While the velocity profile compares well with Krauss and Meyer, there is clearly a difference in the temperature profile.

Table 2.1 summarizes the constants for the velocity law of the wall obtained by various authors. Table 2.2 summarizes the constants for the temperature law of the wall.

It is concluded that a velocity law of the wall close to the form $u^+ = 2.5 \ln y^+ + 5$ is appropriate in axial flow through rod bundles. There is disagreement between investigators, however, as to the law of the wall for temperature.

Table 2.1: Velocity Laws of the Wall

Author	Geometry	Law of the Wall Constants	
		κ	C_1
Hishida and Nagano [6]	circular pipe	0.4	5.5 (no heat)
		0.4	4.65 (heat)
Krauss and Meyer [4]	rod-wall subch.	0.4	5
Meyer [5]	triangular subch.	0.4	5
Rehme [7]	rod-wall subch.	0.4	5.0

Table 2.2: Temperature Laws of the Wall

Author	Geometry	Law of the Wall Constants	
		C_2	C_3
Hishida and Nagano [6]	circular pipe	0.46	4.30
Krauss and Meyer [4]	rod-wall subch.	0.27 to	-0.621 to
		0.43	-0.24
Meyer [5]	triangular subch.	0.4	1

2.2.2 Transition to Turbulence

A fundamental requirement for turbulent interchange mixing is the presence of turbulent flow. The presence of turbulence in a particular flow situation must therefore be ensured.

Cheng and Todreas [8] presented pressure drop characteristics for laminar, transitional and fully turbulent flow for hexagonal rod arrays (*i.e.* triangular subchannels) affixed with helical spacers. Despite the use of spacers, their insights into the dependence of onset-of-turbulence on the pitch-to-diameter ratio, γ_p , is useful. A value of $\gamma_p = 1.1$ represents tightly packed rods typical of many bundle designs. Higher values of γ_p characterize bundles with wider-spaced rods.

Cheng and Todreas found decreasing γ_p increased the Reynolds number value of the onset and duration of the turbulent transition region. For a γ_p of 1.1, turbulence transition began at a Reynolds number of 1.5×10^3 with full turbulence occurring at 1×10^4 . The criteria for fully turbulent conditions is the observation of a pressure drop weakly dependent on Reynolds number.

2.2.3 Turbulent Friction Factor for Fully Developed Flow

The axial pressure gradient, $\Delta p/l$, can be expressed in terms of a Fanning¹ friction factor, f , by balancing the pressure force acting on a fluid volume with the shear force acting on the sides of the volume [2].

$$\frac{\Delta p}{l} = \frac{2\rho f U^2}{D_h} \quad (2.7)$$

where,

$$f = \frac{\tau_w}{\frac{1}{2}\rho U^2} \quad (2.8)$$

The friction factor, f , is a function of both Reynolds number and rod bundle geometry.

Colebrook provides an implicit friction factor expression for friction in a circular pipe [9]:

$$f = \left[-1.738 \ln \left(\frac{e}{3.7} + \frac{1.2615}{\text{Re}\sqrt{f}} \right) \right]^{-2} \quad (2.9)$$

The pipe roughness, e , is zero for smooth pipes.

Although obtained from smooth pipe data, the Colebrook equation (or the Moody diagram equivalent) predicts friction factors higher than that for bare rod geometries with the same hydraulic diameter. This was found to be the case by Meyder [10] for hexagonal bundles and Seale [11] for rod-wall geometries.

Cheng and Todreas [8] present a bare rod friction factor for fully turbulent flow. Given pitch-to-diameter ratio γ_p , the Fanning friction factor is given by the following.

$$f = \left[a + b_1 (\gamma_p - 1) + b_2 (\gamma_p - 1)^2 \right] \text{Re}^{-0.18} \quad (2.10)$$

The -0.18 exponent on Reynolds number was obtained empirically and found to be applicable to both bare and wire wrapped bundles, and is independent of pitch-to-diameter ratio. The constants a , b_1 , and b_2 are a function of bundle geometry and γ_p . The friction factors predicted by Cheng and Todreas and others for a Reynolds number of 10^5 are illustrated in Figure 2.1. The discontinuity in Cheng and Todreas' correlation at $\gamma_p = 1.1$ is an artifact of their choice of fitting parameters. For $\gamma_p < 1.1$, they utilize a strongly quadratic relationship, while for $\gamma_p > 1.1$, they utilize a more linear relationship. Their choice of parameters, however, are not continuous at this junction.

Mohanty and Sahoo [12] found the friction factor for a bundle decreased with decreasing γ_p , however the Reynolds number dependence was constant, very close to that of Blasius' correlation for smooth pipes: $f = 0.0791 \text{Re}^{-0.25}$ (referenced in Schlichting [13]).

¹Some authors use a D'Arcy friction factor, λ , which is exactly four times larger than the Fanning friction factor.

Figure 2.1: Fanning Friction Factor

Blasius, however was found to underpredict the friction factor by approximately 10%. These conclusions are supportive of the Cheng and Todreas curve in Figure 2.1.

Rehme [14] performed a detailed survey of pressure drop data for hexagonal bundles (within which triangular subchannels are found). Rehme founded his friction factor expression on Nikuradse's friction factor, f_{nik} , for a smooth annulus. Nikuradse's friction factor is given by the following implicit formula.

$$\frac{1}{\sqrt{f_{nik}}} = 2.035 \log Re \sqrt{f_{nik}} - 0.989 \quad (2.11)$$

A calibration annulus was used to relate the pitch-to-diameter ratio of a hexagonal array to an equivalent round tube. The radius of the equivalent tube was calculated such that the location of maximum velocity (*i.e.* location of zero shear) corresponded to the position of zero shear in an annulus. From this Rehme obtained the following.

$$f = \begin{cases} f_{nik} [1.045 + 0.071(\gamma_p - 1)] & ; \text{ } Re = 10^4 \\ f_{nik} [1.036 + 0.054(\gamma_p - 1)] & ; \text{ } Re = 10^5 \end{cases} \quad (2.12)$$

Rehme's friction factor curve is shown in Figure 2.1. While Cheng and Todreas' curve suggests friction factors less than that of Nikuradse's and Colebrook's correlation for

circular pipes, Rehme finds the opposite. It must be noted that Cheng and Todreas investigated both bare and appendaged bundles, while Rehme used data for appendaged bundles only. It is expected that bundles with flow-disrupting and turbulence-enhancing appendages would exhibit higher friction than bare bundles and circular pipes.

Inspecting Figure 2.1, both Rehme and Cheng and Todreas assert similar dependence on γ_p for pitch-to-diameter ratios greater than 1.1, although Rehme predicts higher friction. Less than 1.1, however, Cheng and Todreas find a significant drop in friction, while Rehme does not. Very few of Rehme's datasets, however, utilize pitch-to-diameter ratios less than 1.1.

Renksizbulut and Hadaller [15] used Rehme's equivalent annulus and found that the friction factors predicted for a round pipe were lower than that measured in bundles with square lattices. This is similar to Rehme's finding for hexagonal lattices.

The literature review reveals the friction factor is dependent on both Reynolds number and pitch-to-diameter ratio. Further, friction factor correlations for circular pipes are not directly applicable to rod bundle geometries. Given the same hydraulic diameter, bare bundle friction factors are less than that of circular pipes, while appendaged bundle friction factors are higher.

2.2.4 Turbulent Velocity Fluctuations

Rehme [16] performed measurements of the velocity fluctuations in a geometry consisting of a row of rods placed near a straight wall. The pitch-to-diameter ratio, γ_p , was 1.148.

Rehme observed the fluctuations of axial velocity, u' , and velocity parallel to the rod and wall surfaces², v' . The spatial distribution of u' and v' is shown schematically in Figure 2.2. The numbers in the figure represent Rehme's measurements scaled to the friction velocity, u_τ . Rehme provides too many data points to conveniently show in Figure 2.2.

Referring to Figure 2.2, the maximum axial velocity fluctuations are not in the gaps, but rather just outside the narrowest part of the gap. Further, u' is higher near the rod and wall surfaces than in the core of the flow. Circumferentially around the rod, near the surface³, the axial velocity fluctuations varied from a minimum of $2.05u_\tau$ at $\theta = 40^\circ$ to a maximum of $2.45u_\tau$ at $\theta = 70^\circ$. The minimum intensity area was observed in the widest part of the subchannel.

²Rehme uses w' to represent velocity fluctuations parallel to the surfaces, but this is confusing with this investigation's later use of w' to represent the turbulent mixing parameter. Instead, v' is used here to represent the velocity fluctuations parallel to the rod surfaces

³Rehme measured to within 5% of the gap size from the rod wall.

Unlike u' , the maximum parallel velocity fluctuations, v' , were found in the gap centres. The normalized values of v' were roughly 30% lower than comparable values of u' . Further, the normalized value of v' near the rod surface was virtually uniform with a value of $1.6u_\tau$.

In addition to these results, Rehme calculated the turbulence intensity, $\sqrt{u'^2}$ both axially and parallel to the rod surface. Consistent with the velocity fluctuation measurements shown in Figure 2.2, the peak axial turbulence intensities were not observed in the gaps, but rather in a regions at $\theta = 20^\circ$ and $\theta = 70^\circ$. The minimum intensity was observed in the widest part of the subchannel.

The peak parallel turbulence intensity, $\sqrt{v'^2}$, on the other hand, was observed in the narrowest part of the gaps. As with the axial turbulence intensity, the minimum was observed in the widest part of the subchannel.

Rehme also compared his turbulence intensities to Lawn's equation (referenced in [16]) applicable to a circular pipe. In general, the maximum turbulence intensities for the rod-wall geometry were 80 to 120% larger than Lawn's for $\gamma_p = 1.11$. Only in the minimum intensity region in the widest part of the subchannel are Rehme's turbulence intensities close to Lawn's, yet are still 30% higher.

By varying the pitch-to-diameter ratio, γ_p , Rehme observed that both the axial and

parallel turbulence intensities increase with decreasing γ_p (*i.e.*, tighter packed rods). The most pronounced increase in turbulence intensity was observed in the regions of maximum intensity, while the minimum intensity regions changed far less.

Using a rod-wall geometry similar to that of Rehme, Hishida and Nagano [6] measured the turbulence intensity spectrum. The peak turbulence intensity in the near the rod surface was observed at a frequency of 400 Hz. The velocity fluctuations followed a $k_w^{-5/3}$ dependence on wave number, k_w , as predicted by Kolmogorov [17]. The temperature fluctuations followed a similar $k_w^{-5/3}$ dependence.

2.2.5 Wall Shear Distribution

Cararjilescov and Todreas [18] report experimental and theoretical circumferential wall shear variation in a triangular subchannel with $\gamma_p = 1.1$, as shown in Figure 2.3. The experiment indicated that the wall shear was a minimum in the gap with a value of approximately 0.91 of the average wall shear, $\overline{\tau_w}$. The maximum wall shear of approximately $1.07\overline{\tau_w}$ occurred at the $\theta = 30^\circ$ position as measured with $\theta = 0^\circ$ corresponding to the rod-rod gap. For a larger pitch-to-diameter ratio, $\gamma_p = 1.217$, experimental data suggests the circumferential variation in wall shear is more uniform: the minimum value in the gap is $0.97\overline{\tau_w}$ and the maximum is $1.02\overline{\tau_w}$. In addition, the position of maximum wall shear for the $\gamma_p = 1.217$ occurs at $\theta = 20^\circ$. In both cases, the position of local wall shear equaling average wall shear is between $\theta = 10^\circ$ and $\theta = 15^\circ$. Experimental uncertainty is not provided.

Meyer [5] performed similar detailed measurements of velocity in a triangular subchannel. The wall shear varied from $0.91\overline{\tau_w}$ in the rod-rod gap to a maximum of $1.06\overline{\tau_w}$ at an angle of approximately 25° from the rod-rod gap. Meyer also provides error bars of approximately $\pm 0.02\overline{\tau_w}$ on the wall shear distribution.

Renksizbulut and Hadaller [15] observed wall shear distribution results for square subchannels which were similar to those obtained by Meyer. In separate investigations, Rehme [19] and Trupp and Azad [20] also measured circumferential variation of wall shear. Both found similar results: the wall shear is minimized in the gaps and maximized on the surface of the wall which faces directly into the ‘core’ of the subchannel.

Meyer [5] observed that theoretical approaches to wall shear distributions such as that employed by Cararjilescov and Todreas [18] predict maximum wall shear at $\theta = 30^\circ$. Other investigators, however, such as Krauss and Meyer [4], Hooper and Rehme [21] and Seale [22] showed maximum wall shear at higher values of θ . Rapley and Gosman [23] asserted that secondary flows were accountable for this discrepancy between the theoretical

Figure 2.3: Distribution of Wall Shear on Rod Surface (triangular rod geometry)

and observed positions of maximum wall shear. Bartzis and Todreas [24], on the other hand, utilized anisotropy of the turbulent eddy diffusivity to account for the discrepancy. Further discussion on turbulent eddy diffusivity anisotropy is provided in the next subsection, while secondary flows are discussed in Section 2.5. Trupp and Aly [25] use both secondary flow and anisotropic turbulent eddy viscosity models to recreate observed wall shear distributions.

Krauss and Meyer [4] measured velocity fluctuations at 636 positions in the subchannel formed by a rod near a wall ($\gamma_p = 1.12$, $Re = 6.5 \times 10^4$). As shown in Figure 2.4, the circumferential wall shear around the rod was found to vary from a minimum of $0.84\overline{\tau_w}$ in the rod-wall gap and a maximum of $1.16\overline{\tau_w}$ at an angle of 40° from the gap between rods. This position of maximum wall shear is farther from the rod gap than observed by Carajilescov and Todreas and Meyer. In the rod-rod gap itself, the wall shear was measured as $0.97\overline{\tau_w}$.

Rehme [7] measured wall shear in a geometry similar to Krauss and Meyer (Figure 2.4). For a $\gamma_p = 1.07$ and a Reynolds number of 8.7×10^4 , Rehme found a wall shear distribution very similar to that of Krauss and Meyer. Both the Rehme and Krauss and Meyer data shown in Figure 2.4 were adjusted to have an average wall shear value of 1.0

Figure 2.4: Distribution of Wall Shear on Rod Surface (rod/wall geometry)

instead of a maximum wall shear value of 1.0.

2.2.6 Turbulent Eddy Diffusivity Anisotropy

Eddy diffusivity, or viscosity, models of turbulence relate Reynolds turbulence stresses to bulk flow shear by means of a variable turbulent diffusivity of momentum, ϵ_M , or heat, ϵ_H [17]. Section 3.1.5 in Chapter 3 discusses eddy viscosity models in greater detail. Isotropic models assume, at a given location in the flow, the turbulent diffusivity is the same for turbulence behaviour in all directions. Anisotropic models, on the other hand, allow for different values of turbulent diffusivity at a given location for turbulence behaviour in various directions.

Some authors (*e.g.* Hetsroni, Leon, and Hakim [26]) site early work by Elder [27] which revealed the lateral turbulent diffusion coefficient in an open channel is three times higher than that predicted by an assumption of isotropy. Elder found the diffusion of a scalar in a direction perpendicular to that of the main flow is considerably higher than axial diffusion. Using this finding, Hetsroni *et al.* concluded that turbulent diffusion, and therefore mixing, cross-wise to the flow is similarly enhanced.

Later investigators found similar directional dependence of turbulent diffusion. In terms of an eddy diffusivity model of turbulence, this directional dependence can be considered as an anisotropic value of turbulent eddy diffusivity. In other words, ϵ_M and ϵ_H have different values in the axial, radial, and azimuthal directions.

Rehme [16] defines the axial, radial, and azimuthal components of turbulent eddy diffusivity as follows.

$$\epsilon_M^x = \frac{-\overline{u_x'^2}}{\partial U_x / \partial x} \quad (2.13)$$

$$\epsilon_M^r = \frac{-\overline{u_z' u_r'}}{\partial U_r / \partial r} \quad (2.14)$$

$$\epsilon_M^\varphi = \frac{-\overline{u_z' u_\varphi'}}{\partial U_\varphi / \partial \varphi} \quad (2.15)$$

In the azimuthal direction (*i.e.* circumferentially around the rod), Krauss and Meyer [4] found ϵ_M^φ was far greater (by a factor of 10^2) than ϵ_M^r . The maximum anisotropy (*i.e.* ratio of ϵ_M^φ to ϵ_M^r) was observed in the rod-wall gap and was attributed to “strong pulsations parallel to the wall.” Large scatter was observed due to the very small change in axial velocity in the azimuthal direction ($\partial U_\varphi / \partial \varphi$). Kim and Park [28] make reference to Rehme’s observation that the normalized eddy diffusivity in the radial direction is 10 to 100 times smaller than that of the azimuthal component [29].

The spatial variation in eddy diffusivity of momentum was measured by a number of authors (*e.g.* Mohanty [30], Mohanty and Sahoo [12], Ramm and Johannsen [31] and Meyer [5]). The radial component of eddy viscosity of momentum, ϵ_M^r , was found to increase linearly from zero at the rod wall to a maximum value at approximately $r = 0.2\hat{r}$ where r is the distance from the rod wall and $\hat{r}$ is the distance from the rod wall to a symmetry line. From $r = 0.2\hat{r}$ to $\hat{r}$, ϵ_M^r remains fairly constant for triangular subchannels, but drops slightly for square subchannels. Mohanty reports that ϵ_M^r has a maximum value of $0.11u^+\hat{r}$ for triangular subchannels, with this maximum occurring at $r = 0.5\hat{r}$ and $\epsilon_M^r = 0.1u^+\hat{r}$ at $r = \hat{r}$. On the other hand, square subchannels have a maximum $\epsilon_M^r = 0.9u^+\hat{r}$ at $r = 0.5\hat{r}$ and $\epsilon_M^r = 0.7u^+\hat{r}$ at $r = \hat{r}$. These results are in agreement with Meyer. Mohanty and Sahoo [12] show that Reichardt’s model for ϵ_M^φ in a circular tube better reproduces this dependency than does a $k - l$ one equation eddy viscosity model.

Meyer [5] also measured the variation of radial eddy diffusivity of heat, ϵ_H^r , within the subchannel. The variation of ϵ_H^r against r could be best described as a square-root relationship: $\epsilon_H^r \propto \sqrt{r/\hat{r}}$. The maximum value of ϵ_H^r occurred at the subchannel symmetry line.

Figure 2.5: Normalized Radial Eddy Viscosity in Rod-Wall Geometry
(Normalized to $\hat{r}$ and U_τ)

Rehme [7, 16, 19] reports the radial component of eddy viscosity, ϵ_M^r , in rod-wall geometries agreed well with Reichardt's model up to the point where Reichardt's model reached a maximum at $r = 0.4\hat{r}$. Figure 2.5 provides Rehme's measurements normalized to $\hat{r}$ and local shear velocity. Rehme's data, unlike that of Mohanty and Sahoo [12] and Meyer [5] however, indicates ϵ_M^r continues to increase beyond $r = 0.4\hat{r}$. This behaviour is seen both near the rod surface and wall surface. While ϵ_M^r is nearly identical at all circumferential rod locations for $r < 0.4\hat{r}$, it varies considerably for $r > 0.4\hat{r}$. Rehme also found the azimuthal component of viscosity, ϵ_M^φ , varied considerably around the rod for all distances from the rod surface. Further, ϵ_M^φ was observed to range from a minimum equal to the average radial eddy viscosity to a maximum nearly 100 times greater. The minimum ϵ_M^φ values occurred in along radii extending into the core of the flow, while the maximum values were found along radii coincident with the gaps.

From these investigations it is clear that the turbulent diffusivity exhibits directional dependencies. The nature of the anisotropy, however, is more complicated than the three-to-one ratio of axial to transverse diffusivity discussed by Elder. In fact, the ratio of azimuthal to radial diffusivity can be as high as 100-to-one.

Table 2.3: Mixing Mechanisms Identified by Rogers and Todreas [32]

	Natural Mixing	Forced Mixing
Non-directional	Turbulent Interchange	Flow Scattering
Directional	Diversion Cross-Flow	Flow Sweeping

2.3 Coolant Mixing Mechanisms

Rogers and Todreas [32] identify four mechanisms which lead to mixing of energy between subchannels: turbulent interchange, diversion cross flow, flow scattering, and flow sweeping.

Turbulent interchange is a mixing mechanism by which coolant momentum and thermal energy are transported amongst the rods due to turbulent fluctuations in the flow.

Diversion cross flow is defined as bulk fluid transport due to equalization of pressure in the bundle. For example, a region of the bundle with tightly packed rods may divert flow to neighbouring regions with wider-spaced rods. Further, density differences between bundle regions (caused by differences in coolant temperature) may result in diversion cross flow.

Flow scattering and flow sweeping are mixing mechanisms which are caused by the presence of flow obstructions such as rod appendages, spacer grids, or end plates. Mixing by flow scattering involves coolant flow being redirected by an obstruction without any particular direction. In contrast, mixing by flow sweeping involves coolant flow being redirected in a specific direction by a particular obstruction.

Rogers and Todreas classify turbulent interchange and diversion cross-flow as ‘natural’ because they arise ‘naturally’ due to the physics of the flow. Conversely, flow scattering and flow sweeping are classified as ‘forced’ as they require the presence of flow obstructions. In addition, Rogers and Todreas categorize the mixing mechanisms as ‘directional’ and ‘non-directional’. Directional mixing mechanisms are characterized by bulk fluid transport in a particular direction. Non-directional mechanisms, on the other hand, do not exhibit bulk fluid transport in a particular direction.

Table 2.3 summarizes the mechanisms identified by Rogers and Todreas and provides their categorization.

In the absence of flow-disrupting objects such as spacers and other appendages, the two forced mixing mechanisms are not present. Further, in regularly spaced bundles and under conditions of constant density, diversion cross flow is absent. As the current investigation considers bare bundles with constant density, turbulent interchange is the

Figure 2.6: Square, Triangular and Wall Subchannels

primary mixing mechanism.

2.4 Subchannel Models of Coolant Mixing by Turbulent Interchange

2.4.1 Subchannel Approach to Modeling

Simulation tools used by the nuclear safety industry have tended to lump or integrate the modeling of fluid flow through bundles into coarse control volumes or subchannels [1]. A subchannel is defined as the flow area bounded by a cluster of fuel rods. In most rod bundle configurations, three basic subchannel geometries are found: square, triangular and wall (Figure 2.6). The various subchannels in the fuel bundle are laterally connected *via* the small gaps between fuel rods. It is across these gaps that coolant mixing between subchannels occurs. A typical subchannel is less than 10 mm in width with 2 mm wide gaps.

The subchannel approach to coolant mixing represents a relatively coarse discretisation of the domain. This coarse discretisation facilitates rapid solution of the governing equations, a necessity when a transient involving many fuel bundles and thousands of time steps is required. Since relatively large control volumes are used, the fine-grained details of the fluid flow are not resolved, hence constitutive relations are required to provide the information lost in the discretisation process. These constitutive equations include friction factors, k-factors for hydraulic loss, and correlations for turbulent thermal mixing.

2.4.2 Subchannel Models for Turbulent Interchange Mixing

The fundamental assumption of turbulent interchange correlations is that coolant enthalpy is transferred through a gap due to turbulent fluctuations without net transfer of coolant. A common method of modeling this turbulent interchange is through use of the concept of turbulent eddy diffusivity.

Consider two subchannels, i and j , with bulk enthalpies of h_i and h_j , respectively. Let q'' represent the heat flux across a gap of width b due to turbulent interchange. This heat transport is modeled as a diffusive process, using turbulent eddy diffusivity of heat, ϵ_{ij}^H , as the diffusion constant [33].

$$q'' = -\rho\epsilon_{ij}^H \left(\frac{d\bar{h}}{dz} \right)_{ij} \quad (2.16)$$

The negative sign appears because the heat transfer occurs in the direction of decreasing specific enthalpy, which is valid under circumstances of relatively constant heat capacity⁴.

The gradient $(d\bar{h}/dz)_{ij}$ represents the enthalpy gradient across the gap. This is linearized based upon the assumption that the gradient in the gap is equivalent to the difference between the enthalpies of the two subchannels divided by a characteristic distance z_{ij} . Authors often use the centroidal distance between two subchannels, δ_{ij} , as the value of z_{ij} .

$$\left(\frac{d\bar{h}}{dz} \right)_{ij} \simeq \frac{h_j - h_i}{\delta_{ij}} \quad (2.17)$$

Hence, a discrete equation for heat transfer between subchannels due to turbulent interchange mixing is obtained.

$$q'' = -\rho\epsilon_{ij}^H \frac{h_j - h_i}{\delta_{ij}} \quad (2.18)$$

A number of different models have been developed which strive to capture the magnitude of turbulent interchange mixing for a wide range of conditions. One approach is to estimate a value for the turbulent eddy viscosity, ϵ_{ij}^H . A convenient non-dimensionalisation of ϵ_{ij}^H is obtained by dividing by the molecular kinematic viscosity, ν .

An alternative model utilizes a turbulent mixing parameter, w'_{ij} . The mixing parameter is defined to relate the enthalpy difference between channels i and j to the turbulent interchange heat flux per unit length through a gap of width b [33, 32].

$$q''b = w'_{ij} (h_i - h_j) \quad (2.19)$$

⁴Heat transfer occurs in the direction of decreasing *temperature* rather than specific enthalpy (consider warm air being cooled by cooler water). If the heat capacities are equal however, the direction of decreasing enthalpy is equivalent to that of temperature.

The physical interpretation of w' is it represents the amount of mass flow per unit length which would have to take place in order to obtain the observed heat transport due to mixing. In other words, w' is a fictitious mass flow which is equal to the 'real' mass transfer which would be needed to carry the observed amount of heat from one subchannel to another.

Equating Equation (2.19) to Equation (2.18) and substitution of the definition of w' yields the following.

$$\frac{w'_{ij}}{b} (h_j - h_i) = -\rho \epsilon_{ij}^H \frac{h_i - h_j}{\delta_{ij}} \quad (2.20)$$

This provides a relation between the turbulent mixing parameter, w'_{ij} and the eddy diffusivity of heat.

$$w'_{ij} = \rho b \frac{\epsilon_{ij}^H}{\delta_{ij}} \quad (2.21)$$

From Equation (2.21) it can be deduced that w' has a functional dependence on Reynolds number similar to ϵ_{ij}^H .

A third model employs the concept of a gap Stanton number, St_g . The gap Stanton number is defined as the ratio of the turbulent mixing heat transfer through the gap, h_g , to the heat capacity of the axial flow, $\rho c_p U_b$ where U_b is the bulk velocity.

$$\begin{aligned} St_g &= \frac{h_g}{\rho c_p U_b} \\ &= \frac{q'}{b(T_b^i - T_b^j) \rho c_p U_b} \end{aligned} \quad (2.22)$$

The temperatures T_b^i and T_b^j correspond to the bulk temperatures of subchannels i and j , respectively. A larger gap Stanton value represents greater cross-flow turbulent interchange mixing relative to axial convection.

The gap Stanton number can also be written in terms of Nusselt, Reynolds, Prandtl, and Peclet numbers.

$$\begin{aligned} St_g &= \frac{Nu}{RePr} \\ &= \frac{Nu}{Pe} \end{aligned} \quad (2.23)$$

From the above relations it is apparent the gap Stanton number incorporates ratios of axial inertia forces to viscous forces, momentum diffusivities to thermal diffusivities, and dimensionless heat transfer across the gap.

2.4.3 Additional Mixing Models

Aside from the ϵ_{ij} , w'_{ij} and St_g models, investigators have presented additional models which strive to capture a wider range of observed turbulent interchange behaviour.

Rogers and Todreas [32], Rogers and Rosehart [34], and Van Der Ros and Bogaardt [35] define a mass Stanton number as a turbulent interchange mass flux, w'/b divided by axial mass flux ρU .

$$M_{ij} = \frac{w'}{b\rho U} \quad (2.24)$$

Mass Stanton numbers are analogous to gap Stanton numbers: while gap Stanton numbers relate gap heat transfer to axial thermal inertia, mass Stanton numbers relate effective turbulent gap mass transfer to axial mass inertia. Mass Stanton numbers exhibit a Reynolds number dependence similar to gap Stanton numbers.

Rowe and Angle (referenced by Rogers and Todreas [32]) define a mixing parameter β as a mass Stanton number, M_{ij} , scaled by the ratio of the average mass flux in subchannels i and j to the mass flux in subchannel i alone.

$$\beta = M_{ij} \frac{\frac{1}{2}(\rho_i U_i + \rho_j U_j)}{\rho_i U_i} \quad (2.25)$$

The physical interpretation of β is that it is a mass Stanton number scaled to account for increased mixing due to mass flux differences between adjacent subchannels. In situations where density differences between adjacent subchannels are significant (*i.e.* in circumstances of large temperature gradients), β , it is presumed, will provide a more accurate measure of subchannel mixing than M_{ij} alone.

The diversion cross-flow mixing mechanism is accounted for by β models. As discussed previously, in the absence of density differences and in regularly-spaced bundles, diversion cross flow is absent. These conditions also suggest $\rho_i = \rho_j$ and $U_i = U_j$. Thus, in the absence of diversion cross flow, $\beta = M_{ij}$.

The functional dependency of β on Reynolds number should be the same as that for mass and gap Stanton numbers. Castellana, *et al.* [33] found this to be the case. Roidt *et al.* [36], however, calculated a constant value of β , independent of Reynolds number.

Rather than introduce additional mixing mechanisms, these models attempt to combine ϵ_{ij} , w'_{ij} , and St_g models into more ‘universally applicable’ forms. To study the fundamental physics of turbulent interchange mixing, however, consideration of ϵ_{ij} , w'_{ij} , and St_g models alone is sufficient.

2.4.4 Comparison of Mixing Models

The three models, ϵ_{ij} , w'_{ij} , and St_g , are interchangeable.

$$\begin{aligned}\epsilon_{ij}^H/\nu &= \frac{\delta_{ij} w'_{ij}}{\mu b} \\ &= \frac{Re \delta_{ij}}{D_h} St_g\end{aligned}\quad (2.26)$$

$$\begin{aligned}w'_{ij} &= \frac{b\mu}{\delta_{ij}} \epsilon_{ij}^H/\nu \\ &= \frac{Re b \mu}{D_h} St_g\end{aligned}\quad (2.27)$$

$$\begin{aligned}St_g &= \frac{D_h}{Re \delta_{ij}} \epsilon_{ij}^H/\nu \\ &= \frac{D_h}{Re b \mu} w'_{ij}\end{aligned}\quad (2.28)$$

In order to compare the various integrated turbulent interchange models provided by different authors, the above equations have been used to convert the w'_{ij} and St_g models into a common ϵ_{ij}^H/ν format. Table 2.4 provides a summary of these models and indicates (a) which geometry the model is applicable to, and (b) which format the author's model was originally presented.

Table 2.4: Models of Turbulent Interchange

Author	Geometry					Form of integrated model
	Triangle	Square	Triangle-square	Full bundle	Other	
Turbulent Eddy Viscosity, ϵ_{ij}^H , Models						
Cheng and Todreas [8]		● ⁵				$\epsilon_{ij}^H/\nu = 0.0016\text{Re}\frac{\delta_{ij}}{D_h}(\gamma_p - 1)^{-0.5}$ $\epsilon_{ij}^H/\nu = 0.0056\text{Re}\frac{\delta_{ij}}{D_h}(\gamma_p - 1)^{-0.3}$
Elder [27]					● ⁷	$\epsilon_{ij}^H/\nu = 0.0115\text{Re}^{0.875}$

⁵wire-wrapped rods

⁶wire-wrapped rods

⁷open channel

Table 2.4: (continued)

Author	Geometry					Form of integrated model
	Triangle	Square	Triangle-square	Full bundle	Other	
Hetsroni, Leon and Hakim [26]		•				$\epsilon_{ij}^H/\nu = 0.0061\text{Re}^{0.98}$
Nikuradse					• ⁸	$\epsilon_{ij}^H/\nu = \frac{1}{20}\sqrt{\frac{f}{2}}\frac{\text{Re}}{\text{Pr}_i}$
Rogers and Rosehart [34]	•	•	•			$\epsilon_{ij}^H/\nu = 0.00885\text{Re}^{0.9}$
Seale [37]					• ⁹	$\epsilon_{ij}^H/\nu = 0.00755\text{Re}^{0.911}$
Van Der Ros and Bogaardt [35]					• ¹⁰	$\epsilon_{ij}^H/\nu = 0.0035\text{Re}$ $\epsilon_{ij}^H/\nu = 0.0084\text{Re}$ $\epsilon_{ij}^H/\nu = 0.05\sqrt{\frac{1}{2}f}\left(6.12\frac{p}{D_h} - 3.03\right)\text{Re}$
Mixing Parameter, w'_{ij} , Models						
Petrunik [38]	•					$\epsilon_{ij}^H/\nu = 0.009\mu\text{Re}^{0.827}$
Rogers and Todreas [32]	•	•	•			$\epsilon_{ij}^H/\nu = \text{Re}\frac{\sqrt{2}}{40}\sqrt{f}$
Rogers and Tahir [39]	•					$\epsilon_{ij}^H/\nu = 0.0018\frac{\delta_{ij}}{b}\text{Re}_i^{0.9}(\gamma_p - 1)^{-0.40}$ $\epsilon_{ij}^H/\nu = 0.0050\frac{\delta_{ij}}{b}\text{Re}_i^{0.9}(\gamma_p - 1)^{0.106}$ $\epsilon_{ij}^H/\nu = \xi 0.0027\frac{\delta_{ij}}{b}\text{Re}_i^{0.9}(\gamma_p - 1)^{0.050}$ $\xi = \left 1 + \left[\frac{1.101\gamma_p^2 - 1}{1.273\gamma_p^2 - 1}\right]^{1.5}\right $
Rogers and Rosehart [34]				•		$\epsilon_{ij}^H/\nu = 0.0113\text{Re}^{0.875}$

⁸circular pipe⁹effective diffusivity midway between two plates¹⁰gap between square ducts

Table 2.4: (continued)

Author	Geometry					Form of integrated model
	Triangle	Square	Triangle-square	Full bundle	Other	
Roidt <i>et al.</i> [36]	•					$\epsilon_{ij}^H/\nu = 0.00011 \frac{\delta_{ij}}{\mu b} \text{ to } 0.00226 \frac{\delta}{\mu b}$
Rowe [38]		•				$\epsilon_{ij}^H/\nu = 0.0038 \frac{\delta_{ij}}{b} \text{Re}^{0.9}$
Gap Stanton, St_g , Models						
Rapier [40]	•	•				$\epsilon_{ij}^H/\nu = \frac{1}{20} \sqrt{\frac{f}{2}} \frac{\delta_{ij}}{D_h} \text{Re} \left(\frac{\gamma_p - 1}{\gamma_p} \right)$ $\epsilon_{ij}^H/\nu = \frac{1}{10\sqrt{3}} \sqrt{\frac{f}{2}} \frac{\delta_{ij}}{D_h} \text{Re} \left(\frac{\gamma_p - 1}{\gamma_p} \right)$
Rogers and Todreas [32]	•	•	•			$\epsilon_{ij}^H/\nu = \frac{1}{20} \sqrt{\frac{f}{2}} \frac{\delta_{ij}}{D_h} \text{Re} \left(\frac{\gamma_p}{\gamma_p - 1} \right)$
Seale [41]		•	•			$\epsilon_{ij}^H/\nu = 0.004 \left(\frac{1}{\gamma_p - 1} \right) \delta_{ij} \text{Re}^{0.9}$
Seale [37]	•					$\epsilon_{ij}^H/\nu = 0.02968 \frac{\delta_{ij}}{D_h} \text{Re}^{0.9}$

Figures 2.7, 2.8, and 2.9 provide plots of ϵ_{ij}^H/ν for square, triangular, and ‘mixed’ geometries, respectively using a Reynolds number of 10^5 . Mixed geometries are those which the author indicates are appropriate for square, triangular, and other subchannel geometries. The friction factor correlation used to generate these graphs is that of Cheng and Todreas [8], Equation (2.10).

From Figures 2.7 through 2.9, it is clear that a wide range of mixing values exist. The differences between models is more pronounced for smaller values of γ_p . For mixed subchannel geometries (Figure 2.9), Rogers and Todreas’ St_g model predicts mixing far greater than any other model, even Moyer’s w'_{ij} model provided in the same reference. The original form of Rogers and Todreas’ St_g model is as follows.

$$St_g = \frac{1}{20u^+} \left(\frac{\gamma_p}{\gamma_p - 1} \right) \quad (2.29)$$

The simplicity of the model, while perhaps justifiable for large values of γ_p , does not compare well to other models for smaller values of γ_p . Further, the date of Rogers and Todreas’ reference (1968) suggests the St_g model presented in Figure 2.9 represents an early effort at obtaining a mixing model applicable to a wide range of geometries.

Figure 2.7: Turbulent Interchange Models for Square Subchannels

2.4.5 Dependence of Mixing on Pitch-to-Diameter Ratio, γ_p

Comparing Figures 2.7, 2.8 and 2.9, only Rapier's [40] models and Rogers and Todreas' [32] w'_{ij} model for mixed geometries exhibits a decrease in mixing with a decrease in pitch-to-diameter ratio, γ_p . Kim and Park [28] argue that if turbulent interchange is the dominant process in bundle mixing, the mixing rate should be proportional to the relative gap size, $b/D = \gamma_p - 1$. Rapier [40] postulated that, intuitively, turbulent mixing should decrease with the gap size. Only Rapier's and Rogers and Todreas' models, however, exhibit this behaviour.

Besides the other correlations presented in Table 2.4, Hooper's experimental observations suggest otherwise [42]. For $\gamma_p < 1.2$, the product $u_\tau St_g$ rises dramatically, yet is fairly constant for $\gamma_p > 1.2$, particularly for square subchannels. Rapier suggests an interesting analogy to the nautical "harbour paradox", in which the narrowing of a harbour entrance leads to a surprising increase in harbour surging.

The observed increase in mixing as γ_p decreases may be due to an increase in turbulence intensity in the gap observed by Rehme [16] (Section 2.2.4). Ingesson and Kjellström [43] argue that while other phenomena *may* be the source of observed increase in mixing as γ_p decreases, turbulent interchange as the dominant mechanism could not be

Figure 2.8: Turbulent Interchange Models for Triangular Subchannels

precluded. Nevertheless, in the same reference Ingesson and Kjellström concede that net cross-flows of mass through the gap (*i.e.* secondary flow) *may* contribute to mixing. This possibility is discussed in the next subsection.

2.5 Contribution of Secondary Flow to Mixing

Gosman and Rapley [44] observed that analysis of many flows work well by applying equivalent hydraulic diameters to correlations developed for circular ducts. A feature, however, of turbulent flow in non-circular passages which is absent in circular cross-sections is 'secondary' flows generated in the cross-sectional plane. Appendix A provides a discussion of the physical processes which create secondary flows. Using Prandtl's secondary flow categorization (as explained in Appendix A), secondary flows of the second kind are of interest to bundle studies. These secondary flows of the second kind maintain the equilibrium between Reynolds stresses and pressure gradients in the flow.

Gosman and Rapley observe that although secondary flows may have a velocity magnitude of only 1% to 2% of that of the axial velocity, experiment shows secondary flow can have a significant effect on local values of wall shear stress and turbulence proper-

Figure 2.9: Turbulent Interchange Models for Mixed Subchannel Geometries

ties. Wall shear stresses can change by as much as 30% due to secondary flows, while turbulence properties may change by as much as 50%.

Secondary flows of the second kind have been observed or predicted in rod bundle arrays [15, 20, 45]. Rogers and Tahir [39] hypothesize that secondary flow assists in turbulent mixing by reducing the mixing distance as γ_p decreases. They contend that secondary flow is the reason for the counter-intuitive finding that mixing is a weak function of γ_p as observed by many authors. Vonka [46] concludes that secondary flow does not influence momentum and heat transport in the radial direction, but contributes “half of the transport” in the azimuthal direction.

A number of authors, however, (*e.g.* Rehme [16, 29], Seale [37]) observe that secondary flows, although present in bundles, do *not* contribute significantly to subchannel mixing as compared to other mechanisms.

Rehme [29] suggests that the source of the importance of turbulent diffusion anisotropy in rod bundle turbulent transport is the long length scales of turbulent velocity components as compared to the small gap widths.

In a different investigation, Rehme [16] observes that the azimuthal turbulent velocity fluctuation, v' , is not associated with Reynolds-stress driven secondary flow, but rather

by instabilities in the gaps. This is why, Rehme contends, the structure of flow through bundles is different from that of circular pipes, particularly for γ_p less than 1.2.

In yet another study, Rehme [19] argues that the effect of secondary flow on wall shear is rendered inconsequential *if* momentum diffusivity in the azimuthal direction is varied from a maximum value in the gaps to a value 10 to 25 times smaller in the subchannels. This conclusion was based upon observations of model (rather than experimental) behaviour. Specifically, Rehme performed a comparison of experimental results with predictions of the proprietary code, VELASCO.

Meyder [10] found the circumferential variation in rod wall shear was more pronounced with an isotropic turbulent diffusion model as compared to both anisotropic models and experiments. Experimental observation of rod wall shear suggests the isotropic diffusion models overpredict the variation. This also reported by Seale [11] and Mohanty and Sahoo [12].

Bartzis and Todreas [24] agree with Rehme in that turbulent diffusion anisotropy is more responsible for observed cross-flow mixing than is secondary flow. They employed a two-equation eddy viscosity model with different radial and azimuthal turbulent diffusivity values. Secondary flows were modeled by using a choice of two algebraic stress models for the normal turbulence stresses in the radial and azimuthal directions (*i.e.* $\overline{u_r^2}$ and $\overline{u_\theta^2}$). Their results suggest while the use of both anisotropic and secondary flow models produce good results, the use of an anisotropic model alone is quite adequate. Conversely, use of a secondary flow model by itself did not reproduce experimental results as adequately. As with Rehme, it must be emphasized that Bartzis and Todreas conclude that secondary flow is inconsequential compared to turbulence anisotropy based upon results observed before and after invoking numerical models.

Thus, based upon the observations of Rehme, Seale, Meyder, and Bartzis and Todreas, secondary flow does contribute to the observed ‘flattening’ in circumferential wall shear. Indeed, Renksizbulut and Hadaller [15] speculate on the existence of secondary flow based only upon this observed wall shear flattening. Based on observations of *model* performance, however, the contribution of secondary flow to mixing is found to be inconsequential compared to the influence of turbulent diffusivity anisotropy.

2.6 Turbulent Prandtl Number

Nikuradse’s correlation in Table 2.4 includes a turbulent Prandtl number, Pr_t , term which was added to convert Nikuradse’s correlation for eddy diffusivity of momentum to eddy

diffusivity of heat.

$$\text{Pr}_t = \frac{\epsilon_{ij}^M}{\epsilon_{ij}^H} \quad (2.30)$$

While many earlier studies assumed $\epsilon^M \approx \epsilon^H$ (most notably Rogers and Todreas [32]), Krauss and Meyer [4] show that eddy diffusivity of heat in the radial direction is smaller than for momentum, especially in regions close to heated surfaces. The turbulent radial Prandtl number was found to vary between 2 and 2.5, while the turbulent axial Prandtl number was found to be approximately 1. Meyer [5] reports similar results, however the scatter in the turbulent Prandtl number data is quite apparent.

2.7 Influence of Friction Factor on Mixing

The form of Nikuradse's equation in Table 2.4 provides insight into the dependency of eddy diffusivity on Reynolds number. Consider a friction factor equation of the form $f = a\text{Re}^n$. Nikuradse's equation may be written as follows.

$$\begin{aligned} \epsilon/\nu &= \frac{\text{Re}}{20} \sqrt{\frac{a\text{Re}^n}{2}} \\ &= \text{Re}^{1+n/2} \frac{1}{20} \sqrt{\frac{a}{2}} \end{aligned} \quad (2.31)$$

A variety of authors (*e.g.* Cheng and Todreas [8], Blasius [47]) observe that the exponent n is close to a value of -0.2. Hence, ϵ varies with $\text{Re}^{1-0.2/2}$ or $\text{Re}^{0.9}$. This 0.9 dependence is observed in many of results reported in Table 2.4. In other words, models which exhibit a dependency of the form $\text{Re}^{0.9}$ *imply* a friction factor of the form $f = a\text{Re}^{-0.2}$.

The weakest dependence on Reynolds number was given by Petrunik's correlation (reported in Rowe [38]). Elder [27] reports a $\text{Re}^{0.875}$ dependence, while Rogers and Rosehart [34] use Elder's expression and obtain a similar dependence. Elder's correlation, however, was obtained from measurements of an open channel. The strongest Reynolds number dependence of $\text{Re}^{1.0}$ is presented by several investigators. The range of Reynolds number dependency is close to $\text{Re}^{0.9}$ for all models.

2.8 Flow Pulsations in Gap

One model not included in Table 2.4 which requires special discussion is that of Kim and Park [28]. A number of authors (*e.g.* Kim and Park, Möller [48], Wu and Trupp [49], Van der Ros [35]) measured pulsations in the gaps between rods or rods and walls.

Krauss and Meyer [4] state such pulsations are a “general phenomenon of any slot, groove or connecting gap parallel to the flow”. The frequency of the “quasi-periodic” flow pulsations in their hexagonal bundle experiment ($\gamma_p = 1.12$) was measured as 50 to 60 Hz in the rod/rod gaps and 30 to 40 Hz in the rod/wall gaps.

A number of authors employ a Strouhal number to non-dimensionalise gap flow pulsations. The Strouhal number, Sr , is defined in terms of the characteristic pulsation frequency, f_p , rod diameter, D , and friction velocity, u_τ .

$$Sr = \frac{f_p D}{u_\tau} \quad (2.32)$$

Kim and Park [28] cite two Strouhal correlations, one by Möller [48] and one by Wu and Trupp [49]. The Möller correlation has the following form.

$$Sr^{-1} = 0.808 (\gamma_p - 1) + 0.056 \quad (2.33)$$

The Wu and Trupp data suggest the following form.

$$Sr^{-1} = 0.822 (\gamma_p - 1) + 0.144 \quad (2.34)$$

While the dependence on pitch-to-diameter ratio is similar for the two relations, the magnitudes are different. Further, both correlations are independent of the Reynolds number. It is not clear from the references, however, if the Strouhal number is applicable to laminar flow (*i.e.* low Reynolds numbers).

Using arguments that the flow pulsations trace elliptical flow paths in the subchannel gaps, Kim and Park [28] develop a hypothetical path length of the elliptical flow pulsations, z_{FP} , given by the following.

$$z_{FP} = \frac{\pi D}{\sqrt{2}} \left[b_{shape}^2 \left(\frac{\delta_{ij}}{D} \right)^2 + (\gamma_p - 1)^2 \right]^{1/2} \quad (2.35)$$

The shape factor, b_{shape} , reflects the ‘openness’ of the path as seen by the flow pulsation. For square subchannels, a straight line connecting successive subchannel centroids can be drawn without encountering an interfering rod. For a triangular and wall subchannels, however, a straight line connecting successive subchannel centroids will encounter a rod after one or two centroids. As a result z_{FP} is shorter for triangular or wall subchannels than for square. Kim and Park suggest, $b_{shape} = 1$ for square subchannels and $b_{shape} = 2/3$ for triangular subchannels, or subchannels with neighbouring walls.

Given an expression for the friction factor of the form $f = \alpha \text{Re}^n$, Kim and Park report a Stanton number of the following form¹¹.

$$\text{St}_g = \frac{2}{\gamma^2} \sqrt{\frac{\alpha}{2}} \text{Re}^{n/2} \left\{ [1.0 - 0.15 (\gamma_p - 1)] \frac{Z_{FP}}{D} \text{Sr} + \frac{1}{2b_{shape}} \frac{D(\gamma_p - 1)}{\delta_{ij}} \right\} \frac{D_H}{b} \quad (2.36)$$

When converted to an eddy viscosity form, and taking advantage of the relation $b/D = \gamma_p - 1$, Kim and Park's expression becomes as shown.

$$\frac{\epsilon_{ij}}{\nu} = \frac{2}{\gamma^2} \sqrt{\frac{\alpha}{2}} \text{Re}^{1+n/2} \left\{ [1.0 - 0.15 (\gamma_p - 1)] \frac{\delta_{ij} Z_{FP}}{Db} \text{Sr} + \frac{1}{2b_{shape}} \right\} \quad (2.37)$$

Kim and Park suggest using $\gamma = 20$, $\alpha = 0.18$, and $n = -0.2$ as recommended by Rehme [29]. Their model assumes the major axis of the elliptical flow path is equal to the rod pitch, p , while the minor axis is equal to the gap width, b .

Kim and Park's mixing relation yields Stanton number predictions similar to that of other authors. This raises a question about the contribution of gap flow pulsations to coolant mixing. Since Kim and Park's relation provides similar results to those found by other authors, it is concluded that either: (a) the other authors were inadvertently including the effects of flow pulsations when selecting their fitting parameters; or (b) gap flow pulsations do not contribute significantly to mixing and Kim and Park's choice of mixing lengths fortuitously model mixing by turbulent interchange only. It is not clear which of these conclusions is valid.

2.9 Limitations of Integrated Models of Turbulent Interchange Mixing

The limitations of integrated approaches to mixing lie in their reliance upon experimental correlations. While reliance on geometrical factors such as gap width, pitch-to-diameter ratio and hydraulic diameter is expected, dependence on more difficult-to-quantify parameters such as rod configuration is troublesome. This implies that mechanisms which govern subchannel mixing are not easily reduced for a given experiment into universal parameters or the correct basic parameters have not been identified. In other words, it is argued that subchannel mixing is a phenomenon which is quite specific to a particular bundle geometry, and observed mixing behaviour does not scale well into 'lumped' parameters.

¹¹Kim and Park's relation in Reference [28] used the D'arcy friction factor, $\lambda = 4f$.

Of course, development of an integrated mixing model for a particular bundle geometry over an expected range of conditions is certainly useful for simulations involving the given bundle. Extrapolation of conditions outside the empirical range, however, must be performed judiciously.

2.10 Summary

The literature survey has established the following.

1. Coolant mixing in rod bundles involves many phenomena and mechanisms, of which turbulent interchange mixing is one of the more important, particularly in the case of bare rod bundles (*i.e.*, bundles without appendages, *etc.*).
2. A friction factor dependency of the form $f = a\text{Re}^{-0.2}$ is found by most authors. The friction factor for bare rods is usually less than that of a circular pipe of equivalent hydraulic diameter.
3. The velocity law of the wall is applicable to rod bundles with pitch-to-diameter ratios as small as 1.1 for a dimensionless distance-from-the-wall range of approximately $30 < y^+ < 500$. The temperature law of the wall was also found to be applicable, but a wider range of experimental observations were made.
4. The maximum axial velocity fluctuations are observed in the region between the gap and the centroid of the subchannel. The maximum azimuthal velocity fluctuations are observed in the centre of the gap. The turbulent fluctuations increase with decreasing pitch-to-diameter ratio, γ_p .
5. Subchannel, or lumped, models of turbulent interchange exhibit dependencies on subchannel geometry. The Reynolds number dependency, however, is nearly universally equal to $\text{Re}^{0.9}$.
6. Most authors find turbulent interchange mixing is constant for $\gamma_p > 1.5$, but increases as the pitch-to-diameter ratio is decreased. Some authors attribute this to the presence of mass transport by secondary flow. Other argue that turbulent diffusivity anisotropy is more important than secondary flow.
7. The turbulent Prandtl number varies between 2 and 2.5 near the rod walls and close to unity in the core of the subchannels.

Following the literature survey, a number of outstanding questions remain.

First, many subchannel-based correlations assume a friction factor dependency of the form $f = a\text{Re}^{-0.2}$. This assumption is ‘built-in’ to their mixing correlations as exhibited by the dependence of mixing on Reynolds number. The true dependence of both friction factor and mixing on Reynolds number must be determined *independently* of each other. This independence must be obtained in order to verify Nikuradse’s assertion that $\epsilon \propto \text{Re}\sqrt{f}$, the underlying source of the ‘linkage’ between friction factor and mixing.

Second, the dependence of mixing on pitch-to-diameter ratio, γ_p must be verified. Some authors assume or assert that mixing must decrease to zero as $\gamma_p \rightarrow 1$ (*i.e.* the gap between the rods drops goes to zero). Most authors, however, observe that mixing increases as γ_p decreases.

Third, secondary flow has been directly or indirectly observed in rod bundles (based on the distribution of wall shear around the fuel rods). Some investigators (*i.e.* Rehme) contend, however, that the structure of the turbulent flow field, rather than secondary flow, is responsible for the observed wall shear distribution. While the existence of secondary flow is acknowledged, these investigators assert that anisotropy of the turbulent eddy diffusivity is mostly responsible. Turbulent eddy diffusivity, however, is a model rather than a physical quantity. Care must be taken when making arguments about a physical observation such as circumferential wall shear variation based upon the results provided by a mathematical model.

A fourth outstanding question is the role of gap pulsations in coolant mixing. Since many investigators did not explicitly account for such pulsations in their integrated mixing models, the possibility exists that they inadvertently ‘lump’ the effect of gap pulsation mixing into their integrated model.

In order to address these issues, a robust, physically supportable, full-field turbulent interchange mixing model is required. Such a model will provide investigators with a solid basis for comparison of model predictions to experiment. Without a robust full-field turbulent interchange model, it is difficult to separate one mixing effect from another.

The next research task is to establish a model of turbulent interchange mixing and to validate its predictions. The various flow and mixing characteristics discussed in this literature survey will assist in providing a physical basis for development and validation of this model.

Chapter 3

Mathematical Model and Numerical Solution

3.1 Mathematical Model

3.1.1 Instantaneous Quantities and Time Averaging

Five conservation equations are required to model three-dimensional fluid flow and heat transfer: conservation of mass, conservation of momentum in the three coordinate directions, and conservation of energy. Additional equations are required to model the influence of turbulence on the flow and energy fields.

When modeling turbulent flows it is usually necessary to differentiate between instantaneous, quasi-steady, and fluctuating quantities. Instantaneous quantities are those which would be measured by an ideal measuring device placed in the flow; all of the rapid variations in the measured quantity are captured. When modeling turbulence behaviour the instantaneous measurement is often considered as the sum of a slowly varying, time-averaged measurement and a rapidly changing ‘noise’ or fluctuation. For example, instantaneous turbulent velocity, $\tilde{u}_i$, is the sum of a time-averaged component, U_i , and fluctuating component, u'_i .

$$\tilde{u}_i = U_i + u'_i \quad (3.1)$$

Whereas the conservation equations are written in terms of instantaneous quantities, direct modeling of these instantaneous values is often difficult. Instead, the conservation equations are time averaged by means of integration over time. Time averaging is

indicated by an overbar:

$$\begin{aligned}\bar{u}_i &= \frac{1}{\tau} \int_0^\tau (U_i + u'_i) dt \\ &= \bar{U}_i + \bar{u}'_i\end{aligned}\quad (3.2)$$

The integration time, τ , is suitably long enough that U_i is constant but the average of the fluctuating component, u'_i , is zero. The time average $\bar{U}_i$ is simply U_i , while $\bar{u}'_i$ is zero. Hence,

$$\bar{u}_i = U_i \quad (3.3)$$

Instantaneous temperature is indicated by $\tilde{T}$, and is the sum of quasi-steady and fluctuating components. Similarly, instantaneous density and pressure are indicated by $\tilde{\rho}$ and $\tilde{P}$, both of which are also the sum of quasi-steady and fluctuating components.

$$\tilde{T} = T + T' \quad (3.4)$$

$$\tilde{\rho} = \rho + \rho' \quad (3.5)$$

$$\tilde{P} = P + P' \quad (3.6)$$

Since the flows investigated here are incompressible, there are no density fluctuations. Hence $\rho' = 0$ and the instantaneous density, $\tilde{\rho}$ is equal to the quasi-steady density, ρ ; they can be used interchangeably.

While the time average of a fluctuating component is zero, the time average of a product of fluctuating components is non-zero. For example, $\overline{u'_i u'_j}$ is not zero, nor is $\overline{u'_i T'}$. For incompressible flows, however, the fluctuating component of density, ρ' , is zero. Hence time averages of products involving ρ' are zero for incompressible flows. Hence, $\overline{\rho' u'_i}$ and $\overline{\rho' T'}$ are zero for incompressible flows.

3.1.2 Conservation of Mass

Using Einstein summation convention, the instantaneous conservation of mass, also known as the continuity equation, is given by the following [17].

$$\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\tilde{\rho} \tilde{u}_j) = 0 \quad (3.7)$$

Expanding $\tilde{\rho}$ and $\tilde{u}_j$ into their quasi-steady and fluctuating components and time averaging, the following is obtained.

$$\frac{\partial (\bar{\rho} + \overline{\rho'})}{\partial t} + \frac{\partial}{\partial x_j} (\overline{\rho U_j} + \overline{\rho u'_j} + \overline{\rho' U_j} + \overline{\rho' u'_j}) = 0 \quad (3.8)$$

Time averages involving a single fluctuating term are zero. Setting $\bar{\rho} = \rho$ and $\bar{U}_j = U_j$, and recalling that $\rho' = 0$ for incompressible flows, the following is obtained.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j) = 0 \quad (3.9)$$

Since incompressible flows are considered, $\bar{\rho}$ could have been immediately replaced by ρ in Equation (3.7). This will be the convention in subsequent time averaging of equations.

Equation (3.9) can be recast by expanding the second term using the product rule.

$$\frac{\partial \rho}{\partial t} + U_j \frac{\partial \rho}{\partial x_j} + \rho \frac{\partial U_j}{\partial x_j} = 0 \quad (3.10)$$

For incompressible, constant density problems (such as those considered here), the above equation becomes:

$$\frac{\partial U_j}{\partial x_j} = 0 \quad (3.11)$$

This is the time-averaged continuity equation for incompressible flows.

3.1.3 Conservation of Momentum

There are three conservation of momentum equations, one for each coordinate direction, $i = \{1...3\}$. The instantaneous form of the equation for conservation of momentum in the i direction is given by the following [17].

$$\frac{\partial}{\partial t} (\rho \tilde{u}_i) + \frac{\partial}{\partial x_j} (\rho \tilde{u}_j \tilde{u}_i) = -\frac{\partial \tilde{P}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \right] - \rho g_i \quad (3.12)$$

Since incompressible flows are considered, the instantaneous density, $\tilde{\rho}$, has been replaced by its identical time averaged value, ρ (*i.e.* $\rho' = 0$). Equation (3.12) includes a gravitational force, g_i , and molecular dynamic viscosity, μ .

Expanding $\tilde{u}_i$ in Equation (3.12) into its quasi-steady and fluctuating components then time averaging yields the following.

$$\begin{aligned} \frac{\partial}{\partial t} [\rho (U_i + \bar{u}'_i)] + \frac{\partial}{\partial x_j} [\rho (U_j U_i + U_j \bar{u}'_i + U_i \bar{u}'_j + \bar{u}'_i \bar{u}'_j)] = \\ -\frac{\partial}{\partial x_i} (P + \bar{P}') + \frac{\partial}{\partial x_j} \left\{ \mu \left[\frac{\partial (U_i + \bar{u}'_i)}{\partial x_j} + \frac{\partial (U_j + \bar{u}'_j)}{\partial x_i} \right] \right\} - \rho g_i \end{aligned} \quad (3.13)$$

Since time averages involving a single fluctuating velocity are zero, but averages involving two are not, the following is obtained.

$$\begin{aligned} \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_i U_j) + \frac{\partial}{\partial x_j} (\rho \overline{u'_i u'_j}) = \\ -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right] - \rho g_i \end{aligned} \quad (3.14)$$

Rearranging, the term involving $\overline{\rho u'_i u'_j}$ is moved to the right-hand side.

$$\begin{aligned} \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_i U_j) = \\ -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \overline{\rho u'_i u'_j} \right] - \rho g_i \end{aligned} \quad (3.15)$$

This is the incompressible time-averaged form of conservation of momentum in direction i . The Reynolds stress, $\overline{\rho u'_i u'_j}$, requires special treatment, and is discussed further in Section 3.1.5.

3.1.4 Buoyancy Model

Buoyancy forces arise from density gradients caused by temperature changes. Modeling buoyancy is discussed in this subsection.

The pressure in Equation (3.15) can be separated into dynamic, P_d , and hydrostatic components, P_h . The hydrostatic pressure can be expressed as a function of a reference pressure, P_0 , and an average, or free-stream, density, ρ_∞ .

$$\begin{aligned} P &= P_d + P_h \\ &= P_d + \left[P_0 - \int \rho_\infty g dy \right] \end{aligned} \quad (3.16)$$

In the equation above, the integration is performed in the positive y direction. This assumes the gravitational force, g_i , acts in the negative y direction (*i.e.* $i = 2$). Differentiating with respect to the vertical direction, y ,

$$\frac{\partial P}{\partial y} = \frac{\partial P_d}{\partial y} - \rho_\infty g \quad (3.17)$$

Substitution into the time average momentum equation yields the following.

$$\begin{aligned} \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_i U_j) = \\ -\frac{\partial P_d}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \overline{\rho u'_i u'_j} \right] - (\rho - \rho_\infty) g_i \end{aligned} \quad (3.18)$$

Note that in the x and z directions (*i.e.* $i = 1, 3$), the gravitational force, g_i , is zero. Therefore there is no buoyancy force in these directions.

The density difference appearing in the buoyancy force can be related to the temperature field through the volumetric thermal expansion coefficient, β , is defined as follows [50]:

$$\begin{aligned} \beta &= -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_p \\ &\approx -\frac{1}{\rho} \left(\frac{\rho_\infty - \rho}{T_\infty - T} \right) \end{aligned} \quad (3.19)$$

therefore,

$$(\rho_\infty - \rho) \approx \rho\beta(T - T_\infty) \quad (3.20)$$

The Boussinesq approximation states that departures of local density, ρ , from the average density, ρ_∞ , are small [47]:

$$\frac{\rho - \rho_\infty}{\rho_\infty} \ll 1 \quad (3.21)$$

This allows substitution of Equation (3.20) into the time-averaged momentum equation without altering the density in terms other than the term with gravity.

$$\begin{aligned} \frac{\partial}{\partial t}(\rho U_i) + \frac{\partial}{\partial x_j}(\rho U_i U_j) = \\ -\frac{\partial P_d}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \overline{\rho u'_i u'_j} \right] - \beta \rho (T - T_\infty) g_i \end{aligned} \quad (3.22)$$

Given a volumetric thermal expansion coefficient, β , and reference temperature, T_∞ , the buoyancy force is modeled in the time-averaged conservation of momentum equation as a body force.

3.1.5 Eddy Viscosity Model of Turbulence

The main difference between Equation (3.15) and the instantaneous form given in Equation (3.12) (other than the use of U_i instead of $\tilde{u}_i$) is the appearance of the $-\overline{\rho u'_i u'_j}$ term. Called the Reynolds stress, this term arises from convection of momentum by turbulent fluctuations. Calculating the Reynolds stress directly or indirectly and determining its influence on the flow is the driving force behind turbulence modeling and research.

Eddy viscosity models are one class of models that estimate the Reynolds stress field for a given flow. This class of models assumes the Reynolds stress is proportional to the bulk flow strain, with turbulent viscosity, μ_t , as the proportionality constant.

$$-\overline{\rho u'_i u'_j} = \mu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} \quad (3.23)$$

In the form of the equation, above, the turbulent kinetic energy, k , appears in a term which includes the Kroenecker delta function. This appearance is due to the definition of the turbulent kinetic energy.

$$k = \frac{1}{2} \overline{u'_i u'_i} \quad (3.24)$$

Recalling the presence of repeated indices implies summation, addition of Equation (3.23) over $i = \{1...3\}$ yields the following for $i = j$:

$$-\overline{\rho u'_i u'_i} = 2\mu_t \frac{\partial U_i}{\partial x_i} - 2\rho k \quad (3.25)$$

The continuity equation for incompressible flow, however, implies $\partial U_i / \partial x_i = 0$. Without the $2k\delta_{ij}/3$ at the end of Equation (3.23), the physically incorrect result $-\rho \overline{u'_i u'_i} = 0$ would have been obtained from the equation above.

The turbulent eddy viscosity, μ_t , is modeled as being proportional to a characteristic velocity, V , and a characteristic length, l .

$$\mu_t \propto \rho V l \quad (3.26)$$

Dimensional analysis suggests the characteristic velocity should be expressed as proportional to the square root of turbulent kinetic energy. The length scale, also using dimensional arguments, is expressed as proportional to the turbulent kinetic energy and turbulent dissipation rate, ε .

$$V \propto \sqrt{k} \quad (3.27)$$

$$l \propto \frac{k^{3/2}}{\varepsilon} \quad (3.28)$$

$$(3.29)$$

Thus, the turbulent viscosity can be written as follows.

$$\mu_t = \frac{\rho c_\mu k^2}{\varepsilon} \quad (3.30)$$

where the variable c_μ is a constant of proportionality, equal to 0.09 for the current investigation.

The time-averaged momentum equation, therefore, can be written using the turbulent viscosity.

$$\begin{aligned} \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_i U_j) = \\ - \frac{\partial}{\partial x_i} \left(P + \frac{2}{3} \rho k \right) + \frac{\partial}{\partial x_j} \left[(\mu + \mu_t) \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right] - \beta \rho (T - T_\infty) g_i \end{aligned} \quad (3.31)$$

The value of μ_t in Equation (3.30) is the same for all directions, i . In other words, this model is isotropic.

In order to calculate the isotropic turbulent eddy viscosity, μ_t , using Equation (3.30), the k and ε fields must be calculated. This is accomplished using transport equations for these fields, as discussed in the next subsection.

3.1.6 $k - \varepsilon$ Turbulence Model

The transport of turbulent kinetic energy per unit mass, k , in high Reynolds number form, is provided by the following equation [51].

$$\underbrace{\rho \frac{\partial k}{\partial t}}_{\text{I}} + \underbrace{\rho U_i \frac{\partial k}{\partial x_i}}_{\text{II}} = \underbrace{\frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right]}_{\text{III}} + \underbrace{P_k}_{\text{IV}} - \underbrace{\rho \varepsilon}_{\text{V}} + \underbrace{\frac{\rho \mu_t}{\text{Pr}_t} \beta \left(g_i \frac{\partial T}{\partial x_i} \right)}_{\text{VI}} \quad (3.32)$$

Term I is the rate of change of k , while term II is the convection of k . Term III is the diffusion of k , and includes an empirical constant, σ_k . Term IV is the volumetric production of k , and is modeled using the following.

$$\begin{aligned} P_k &= -\overline{\rho u'_i u'_j} \frac{\partial U_i}{\partial x_j} \\ &= \left[\mu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} \right] \frac{\partial U_i}{\partial x_j} \\ &= \left[\mu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right] \frac{\partial U_i}{\partial x_j} - \frac{2}{3} \rho k \frac{\partial U_i}{\partial x_i} \end{aligned} \quad (3.33)$$

The $-\frac{2}{3} \rho k \delta_{ij}$ term disappears from the equation above after application of continuity. Therefore,

$$P_k = \left[\mu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right] \frac{\partial U_i}{\partial x_j} \quad (3.34)$$

Term V is the turbulence dissipation rate per unit mass, where ε is determined using its own transport equation. Term VI is a turbulence source arising from fluid buoyancy and includes the turbulent Prandtl number, Pr_t . The turbulent Prandtl number is equal to the ratio of turbulent diffusivity of momentum to turbulent diffusivity of heat. This model assumes Pr_t is constant and equal to 0.9.

The high Reynolds number form of the transport equation for the turbulence dissipation rate, ε , is given by the following [51].

$$\underbrace{\rho \frac{\partial \varepsilon}{\partial t}}_{\text{I}} + \underbrace{\rho U_i \frac{\partial \varepsilon}{\partial x_i}}_{\text{II}} = \underbrace{\frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right]}_{\text{III}} + \underbrace{\frac{\varepsilon}{k} (c_{\varepsilon_1} P_k - c_{\varepsilon_2} \rho \varepsilon)}_{\text{IV}} \quad (3.35)$$

Term I is the rate of change of ε , while term II is the convection of ε . Term III is the diffusion of ε and includes an empirical constant, σ_ε . Term IV is the source of dissipation and includes two additional empirical constants, c_{ε_1} and c_{ε_2} . The source of dissipation is proportional to the difference between the production and dissipation of turbulent energy.

The empirical constants used in the k and ε equations are summarized in Table 3.1.

Table 3.1: $k - \varepsilon$ Model Constants

c_μ	$c_{\varepsilon 1}$	$c_{\varepsilon 2}$	σ_k	σ_ε	Pr_t
0.09	1.44	1.92	1.0	1.3	0.9

3.1.7 Conservation of Energy

The instantaneous form of the conservation of the energy equation is given by the following [47].

$$c_p \frac{\partial}{\partial t} (\rho \tilde{T}) + c_p \frac{\partial}{\partial x_j} (\rho \tilde{u}_j \tilde{T}) = \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \tilde{T}}{\partial x_j} \right) + \dot{q}''' \quad (3.36)$$

where Γ is the fluid molecular conductivity.

Expanding the instantaneous temperatures and velocities and time averaging yields the following.

$$c_p \frac{\partial}{\partial t} (\rho T) + c_p \frac{\partial}{\partial x_j} (\rho U_j T) = \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial T}{\partial x_j} - \rho c_p \overline{u'_j T'} \right) + \dot{q}''' \quad (3.37)$$

As with the momentum equation, the process of time averaging the energy equation creates a new term, in this case $-\rho c_p \overline{u'_j T'}$. This term is modeled using the turbulent diffusivity of heat, μ_t^H [51].

$$-\rho \overline{u'_j T'} = \mu_t^H \frac{\partial T}{\partial x_j} \quad (3.38)$$

As introduced in the $k - \varepsilon$ turbulence model section, the turbulent Prandtl number, Pr_t , is defined as the ratio of the turbulent viscosity of momentum μ_t , to μ_t^H .

$$\text{Pr}_t = \frac{\mu_t}{\mu_t^H} \quad (3.39)$$

Using this definition of turbulent Prandtl number, and substituting Equation (3.38) into Equation (3.37), the time averaged energy equation can be written as follows.

$$c_p \frac{\partial}{\partial t} (\rho T) + c_p \frac{\partial}{\partial x_j} (\rho U_j T) = \frac{\partial}{\partial x_j} \left[\left(\Gamma + c_p \frac{\mu_t}{\text{Pr}_t} \right) \frac{\partial T}{\partial x_j} \right] + \dot{q}''' \quad (3.40)$$

The term $c_p \mu_t / \text{Pr}_t$ behaves in Equation (3.40) as a turbulent conductivity, Γ_t . Writing $\Gamma_t = c_p \mu_t / \text{Pr}_t$, an alternate expression for Pr_t is obtained.

$$\text{Pr}_t = \frac{c_p \mu_t}{\Gamma_t} \quad (3.41)$$

The time-averaged form of the energy equation can be therefore written as:

$$c_p \frac{\partial}{\partial t} (\rho T) + c_p \frac{\partial}{\partial x_j} (\rho U_j T) = \frac{\partial}{\partial x_j} \left(\Gamma_{eff} \frac{\partial T}{\partial x_j} \right) + \dot{q}''' \quad (3.42)$$

where,

$$\Gamma_{eff} = \Gamma + c_p \frac{\mu_t}{Pr_t} \quad (3.43)$$

3.1.8 Boundary Conditions

In order to solve the governing equations in a given domain, boundary conditions are required. Four main boundary conditions are considered: wall, inlet, outlet, and symmetry.

Wall Boundaries

Walls are stationary and impermeable, thus velocities normal to the wall are zero. Further, a ‘no-slip’ condition is applied at the wall, thus velocities parallel to the wall are zero at the wall. This provides sufficient boundary conditions for the continuity and the momentum equations for laminar flow.

While a zero wall velocity condition for the momentum equation is sufficient for laminar flows, turbulent flows require additional modeling. Very close to the wall viscous forces exceed inertial forces, thus turbulence cannot be maintained, and the flow is laminar. Between this laminar sublayer and the free turbulent flow far from the wall lies a transition or buffer layer and a region of logarithmic velocity increase. The wall boundary condition must account for the influence of these three layers (laminar, buffer, and logarithmic) on momentum transport to the wall. This is achieved by using a law of the wall for the momentum equation’s wall boundary condition.

$$U^+ = \frac{1}{0.41} \ln y^+ + 5.2 \quad (3.44)$$

where $U^+ = U/U_\tau$. The dimensionless distance from the wall, y^+ , is defined in terms of the shear velocity, U_τ and wall distance, y .

$$y^+ = \frac{\rho U_\tau y}{\mu} \quad (3.45)$$

where,

$$U_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad (3.46)$$

A similar law of the wall is used as a boundary condition for the energy equation in turbulent flow. For a specified wall temperature T_w , the wall heat flux, q_w , is given by the following.

$$q_w = \frac{U_\tau}{T^+} (T_w - T) \quad (3.47)$$

where T is the fluid temperature at a near-wall node.

The dimensionless temperature is evaluated using the following [52].

$$T^+ = \text{Pr} y^+ e^{-\Lambda} + [2.12 \ln y^+ + \beta^*] e^{-1/\Lambda} \quad (3.48)$$

$$\beta^* = (3.85 \text{Pr}^{1/3} - 1.3)^2 + 2.12 \ln \text{Pr} \quad (3.49)$$

$$\Lambda = \frac{0.01 (\text{Pr} y^+)^4}{1 + 5 \text{Pr}^3 y^+} \quad (3.50)$$

$$\text{Pr} = \frac{\mu c_p}{k} \quad (3.51)$$

The wall boundary condition for the k and ε equations are based upon three assumptions about the turbulence field:

1. production of turbulence, P_k , equals dissipation, $\rho\varepsilon$;
2. constant shear layer (*i.e.* Couette flow); and
3. the velocity gradient normal to the wall is much greater than the gradient along the wall.

These assumptions, when combined with the law of the wall (Equation (3.44)), yield a near-wall value of ε inversely proportional to the distance from the wall.

$$\varepsilon = \frac{U_\tau^3}{0.41y} \quad (3.52)$$

The production of turbulent kinetic energy, P_k , is calculated using the following, where U_t is the velocity tangential (*i.e.* parallel) to the wall and n is normal to the wall.

$$\begin{aligned} P_k &= \tau_w \frac{\partial U_t}{\partial n} \\ &= \frac{\tau_w^2}{\mu} \frac{dU^+}{dy^+} \end{aligned} \quad (3.53)$$

The gradient dU^+/dy^+ is estimated by differentiation of Equation (3.44).

Inlet Boundaries

The inlet boundary condition for the continuity equation is modeled using a specified inlet velocity.

The inlet condition for conservation of momentum consists of three components: advection of momentum, a pressure force, and a viscous force. The specified inlet velocity is applied to the advection term, while the pressure force is determined by interpolation of the pressure field. The viscous force is estimated from velocity gradients just inside the inlet.

The inlet conditions for the k and ε equations utilize a specified turbulence intensity, T_u , and eddy length scale, L_ε .

$$k = \frac{3}{2} T_u^2 U_b^2 \quad (3.54)$$

$$\varepsilon = \frac{k^{3/2}}{L_\varepsilon} \quad (3.55)$$

The turbulence intensity is usually specified as 5%, while the eddy length scale is specified as equal to a domain characteristic length, such as the radius for flow in a circular pipe. The actual k and ε fields will develop with the flow and are insensitive to the choice of inlet values of T_u and L_ε if the development length is sufficient. Analysis of flows without fully developed conditions will require careful selection of inlet conditions. This is not the case in this investigation, however.

The inlet condition for the energy equation consists of a specified temperature.

Outlet Boundaries

The continuity equation does not require an outlet condition unless the outlet mass flow or velocity is explicitly specified. This is not the case in the current investigation.

The outlet boundary condition for the momentum equation uses a pressure field which is fixed at a single location. The remainder of the outlet pressure field varies such that the pressure at the specified location matches the pre-determined value. The flow of momentum is modeled as purely advective at the outlet.

The outlet condition for the k and ε fields is assumed to be purely advective (*i.e.* the diffusive component is zero). This assumption increases in validity as the outlet approaches fully developed conditions.

The outlet boundary for the energy equation assumes the heat transport is purely advective. This assumption is increasingly valid as the flow becomes fully developed.

Symmetry Boundaries

At a symmetry boundary, fluxes normal to the boundary are zero. Thus for the continuity equation, mass flux across the symmetry boundary is zero. For the momentum equation, momentum flow ($\dot{m}U$) across the boundary is also zero. For the turbulent kinetic energy and dissipation rate, their respective flows ($\dot{m}k$ and $\dot{m}\varepsilon$) normal to the boundary are zero. The heat flow normal to the boundary, like the other conserved quantities, is set to zero normal to the symmetry boundary.

Figure 3.1: Schematic of Two-Dimensional Control Volume

3.2 Numerical Solution

In order to be solved by computer, the continuous-form conservation equations must be recast into sets of discrete algebraic equations. This is accomplished by integrating the differential equations over discrete subcomponents of the solution domain.

Once discretized, boundary conditions are applied, and a solution algorithm is used to solve the complete set of equations.

3.2.1 Discretization of Domain

The solution domain is discretized by defining discrete locations, or nodes, at which the field variables are evaluated. The value at a node is equal to the mean of the field averaged over a small region, or control volume, surrounding the node. The assembled set of control volumes completely fill the solution domain without overlap.

For control volumes which do not touch the boundary of the domain (*i.e.* interior control volumes), the governing node is placed at the geometric centre of the control volume. For control volumes on the domain boundary the governing node is placed at the edge of the control volume, coincident with the boundary.

Figure 3.1 illustrates a two-dimensional control volume, ω_i , showing its governing node, i . Both interior and edge control volumes are shown. Note that although the control volumes in Figure 3.1 are orthogonal, this is not a requirement.

3.2.2 Discretization of Governing Equations

The finite volume approach to discretizing the governing equations involves the integration of the each equation over each discrete control volume, ω_i .

The transport of a general scalar, φ , is expressed by the following.

$$\frac{\partial}{\partial t}(\rho\varphi) + \frac{\partial}{\partial x_j}(\rho u_j \varphi) = \frac{\partial}{\partial x_j} \left[\Gamma_\varphi \left(\frac{\partial \varphi}{\partial x_j} \right) \right] + S_\varphi \quad (3.56)$$

The units of φ are ‘conserved quantity per unit mass’. For the continuity equation, the transported scalar is unity (*i.e.*, φ is ‘mass per unit mass’ or $\varphi = 1$). For momentum, $\varphi = U_i$, while for energy, φ represents enthalpy. The turbulent kinetic energy and dissipation equations can be cast in the form of Equation (3.56) by including the production and dissipation terms in the source term, S_φ .

Consider Equation (3.56) integrated over ω_i :

$$\int_{\omega_i} \frac{\partial}{\partial t}(\rho\varphi) d\omega_i + \int_{\omega_i} \frac{\partial}{\partial x_j}(\rho u_j \varphi) d\omega_i = \int_{\omega_i} \frac{\partial}{\partial x_j} \left[\Gamma_\varphi \left(\frac{\partial \varphi}{\partial x_j} \right) \right] d\omega_i + \int_{\omega_i} S_\varphi d\omega_i \quad (3.57)$$

Integrals in Equation (3.57) which contain a divergence of a vector (*i.e.* a $\partial u_j / \partial x_j$ term) are converted from a volume integral to an integral over surface s using Gauss’ divergence theorem.

$$\int_{\omega_i} \frac{\partial u_j \varphi}{\partial x_j} d\omega_i = \int_s u_j \varphi dn_j \quad (3.58)$$

The scalar n_j represents the component of the outward facing surface normal parallel to x_j . Thus Equation (3.57) is rewritten as follows.

$$\int_{\omega_i} \frac{\partial}{\partial t}(\rho\varphi) d\omega_i + \int_s \rho u_j \varphi dn_j = \int_s \Gamma_\varphi \left(\frac{\partial \varphi}{\partial x_j} \right) dn_j + \int_{\omega_i} S_\varphi d\omega_i \quad (3.59)$$

Discretization of volume integrals in Equation (3.59) is straightforward. The value of φ at nodal point i in control volume ω_i is given by φ_i . Since the nodal value equals the mean value of the scalar over the control volume,

$$\int_{\omega_i} \varphi d\omega_i = \varphi_i V_i \quad (3.60)$$

where V_i is the volume of control volume ω_i .

The time derivative is evaluated by a first-order backward Euler approximation.

$$\frac{\partial}{\partial t}(\rho\varphi) = \frac{\rho\varphi - \rho^o\varphi^o}{\Delta t} \quad (3.61)$$

Integration of surface integrals in Equation (3.59) is somewhat more complex. Fluxes through surfaces are evaluated at integration points which lie on the boundary between

Figure 3.2: Two-Dimensional Finite Elements and Integration Points

control volumes. The placement of integration points is determined based on the definition of finite elements. A finite element is a region of the domain defined by nodes at the corners (Figure 3.2). In two dimensions, an interior finite element overlaps four control volumes. The subset of a control volume which is found in a given finite element is called a quadrant. The integration points are placed at the centre of each outward facing quadrant side. As seen in Figure 3.2, a two-dimensional control volume has eight integration points. As also seen in Figure 3.2, neither the element nor the control volumes are necessarily square.

Using the notation ip to represent an integration point, the surface integral is converted to a summation of calculations at integration points.

$$\int_s \rho u_j \varphi dn_j \approx \sum_{ip} (\rho u_j \varphi \Delta n_j)_{ip} \quad (3.62)$$

The subscript ip indicates that the quantity $\rho u_j \varphi \Delta n_j$ is evaluated at the integration point. The variable Δn_j is the unit normal to the quadrant face containing ip .

An advantage of using integration points to evaluate fluxes across boundaries is that two control volumes which share a common boundary also share identical integration point values. This ensures the flux leaving one control volume is exactly equal to the flux entering the next, thereby providing a strongly conservative solution.

Assembling the terms, the discretized form of the transport equation is written as

follows.

$$V_i \left(\frac{\rho\varphi - \rho^o\varphi^o}{\Delta t} \right)_i + \underbrace{\sum_{ip} (\rho u_j \varphi \Delta n_j)_{ip}}_I = \underbrace{\sum_{ip} \left[\Gamma_\varphi \left(\frac{\partial \varphi}{\partial x_j} \right) \Delta n_j \right]_{ip}}_{II} + S_{\varphi,i} V_i \quad (3.63)$$

Term I is an advection term, while term II is a diffusion term. Both these terms involve evaluation of φ at integration points rather than nodal points.

The diffusion term is evaluated by using an approach based on finite element methods. Shape functions are used to convert gradients of scalar fields into products of shape functions gradients and nodal values of φ .

Evaluation of the advection term is somewhat more complex. While diffusion terms are elliptic, advection terms are hyperbolic. If an elliptic evaluation of advection terms is performed, non-physical results are obtained. The integration point values in the advection term are determined using a type of physical advection correction scheme called the skew upstream differencing scheme. This scheme estimates the integration point values by isolating the advection term of a transport equation along a streamline following the flow.

Appendix B provides details of the evaluation of the diffusion and advection terms at the integration points, including a more detailed description of skew upwind differencing.

3.2.3 Three-Dimensional Representation

The preceding discretization was presented using a two-dimensional domain. Extrapolation to three dimensions is straightforward. Finite volumes, elements, and integration points are defined the same for three dimensional domains as for two dimensional. Instead of integration points being defined on the outward surfaces of quadrants, in three dimensions integration points are defined on the outward surfaces of octants. Given that a control volume is comprised of eight octants with three outward faces on each octant, there are a total of 24 integration points per three dimensional control volume.

The discretization for three dimensions is performed the same as for two. Figure 3.3 illustrates a schematic of an octant, integration points, and finite elements in three dimensions.

3.2.4 Discretization of Boundary Conditions

As with the conservation equations, the boundary conditions must be discretized and applied to the set of algebraic equations to be solved.

Figure 3.3: Three Dimensional Control Volume Octant

Boundary conditions are specified at integration points. For control volumes on exterior boundaries of the domain, integration points are located on the exterior boundary surface.

Wall Boundary

For laminar flow, the no-slip condition is applied by setting the velocity tangential to the wall equal to zero at integration points on the boundary. Similarly, the impermeability condition is applied by setting the velocity normal to the wall equal to zero at the same integration points. The pressure at the integration points is estimated by interpolation of the control volume pressures.

Turbulence flows require additional equations to properly capture the influence of near-wall effects on the flow body. This is accomplished by applying the law of the wall, Equation (3.44), to velocities at nodes near, but not on, the wall boundary. In order to calculate U^+ , the shear velocity, U_τ , and dimensionless distance from the wall, y^+ , must be determined.

The wall shear, U_τ , is determined based on the k value near the wall by assuming that near the wall turbulence production equals dissipation and a constant shear layer is present.

$$U_\tau = c_\mu^{1/4} \sqrt{k} \quad (3.64)$$

The dimensionless distance from the wall to the closest nodes in the flow is calculated using the above value of U_τ .

$$y^+ = \frac{\rho c_\mu^{1/4} \sqrt{k} \Delta y}{\mu} \quad (3.65)$$

where Δy is the distance from the wall to the nearest node in the flow. In order for the law of the wall to be applicable, y^+ must be in the range $30 < y^+ < 300$ [2]. Thus the placement of the first set of nodes in the flow near the wall must be made carefully such that y^+ does not fall outside of its specified range. Since y^+ is a function of the wall shear which in turn is a function of Reynolds number, the placement of the near-wall nodes changes depending upon the Reynolds number of the flow.

The near-wall values of k , ε and $\rho c_p T$ are calculated using the above definitions of U_τ and y^+ in conjunction with Equations (3.52), (3.53) and (3.48).

Inlet Boundary

The inlet boundary for the continuity equation consists of a mass flux evaluated at integration points, $\dot{m}_{ip} = \rho A U_{ip}$, which is calculated using a specified nodal velocity, U_i^{spec} .

$$\dot{m}_{ip} = \rho_{ip} A_{ip} U_i^{spec} \quad (3.66)$$

Inlet boundary values for the momentum equation are also evaluated at integration points. The inlet momentum flow, $\dot{m}_i U_i$, is the sum of advection, pressure, and viscous force components.

$$(\dot{m}U)_i = \underbrace{\dot{m}_{ip} U_i^{spec}}_{\text{advection}} + \underbrace{A_i \sum_n N_n P_n}_{\text{pressure}} + \underbrace{A_j \mu_{ip} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)_{ip}}_{\text{viscous}} \quad (3.67)$$

where $\dot{m}_i = \rho U_i$ and N_n is a shape function at nodal point n .

The inlet boundary conditions for k and ε consist of a specified turbulence intensity, T_u , and length scale, L_ε . These are used to obtain inlet values of k and ε using Equations (3.54) and (3.55) which are substituted into the discretized equations.

The energy equation assumes that inlet heat flow, $\rho c_p U_i T_i$, is advective. A specified inlet temperature is applied to all nodal points and integration points.

Outlet Boundary

The outlet boundary consists of a reference pressure, P^{ref} , specified at a single finite element face on the outlet. This face contains four integration points, ip , and four nodes,

n . The pressure at every integration point on the outlet is calculated using the following.

$$P_{ip} = \sum_n N_n P_n + \underbrace{\left(P^{ref} - \sum_n N_n P_n \right) \Big|_{ip \text{ spec}}}_{\text{correction term}} \quad (3.68)$$

Shape functions at each node location are given by N_n . The correction term represents the numerical difference between the reference pressure and the average pressure over the control volume face at which the reference pressure is specified. As the grid is refined, this term goes to zero. This correction is applied so that the pressure closure is consistent on all boundary faces.

The outlet condition for momentum, k , ε , and energy is pure advection. Thus outlet flows of U_i , k , ε and energy are calculated by multiplying U_i , k , ε , and $c_p T$ by the mass flow calculated at each outlet integration point, $\dot{m}_{ip}$.

Symmetry Boundary

The symmetry boundary condition implies that flows normal to the boundary are zero. Thus total flow of mass, k , ε and energy are zero across a symmetry boundary. This is specified by setting U_{ip} normal to the boundary equal to zero for all integration points on the symmetry boundary.

The symmetry condition for momentum conservation implies that viscous forces parallel to the symmetry boundary are zero. Thus, only a pressure force and normal viscous force remain. Thus, at each symmetry boundary integration point, the symmetry condition for momentum at each integration point is:

$$(\dot{m}_{ip} U_{ip})_i = A_i \sum_n N_n p_n + \left[A_k \mu_{ip} \left(\frac{\partial U_j}{\partial x_k} + \frac{\partial U_k}{\partial x_j} \right) n_j \right] n_i \Big|_{ip} \quad (3.69)$$

where n_i and n_j are unit normals in the i and j directions, and N_n is a shape function at nodal point n .

3.2.5 Grid Colocation

A difficulty associated with solving the momentum and continuity equations is the weak coupling between pressure and velocity fields. Specifically, the discretized form of the continuity equation for a given control volume does not include the pressure at the node within the volume. This can lead to non-physical ‘checkerboarding’ of the pressure field [53].

Some researchers have circumvented this problem by using staggered grids [53, 54, 55] in which pressure is solved on a grid misaligned with the velocity grid. While effective for orthogonal grids (*e.g.* Figure 3.1), grid staggering is difficult when non-orthogonal grids are used (*e.g.* Figure 3.2 or Figure 3.3).

A solution is to solve the discretized equation in a manner which does not suffer from pressure/velocity decoupling, thus removing the need for grid staggering. As discussed in detail in Appendix C, grid collocation is accomplished by splitting the velocity into two calculations, one used to calculate mass flows at a control volume face and one used to calculate momentum flow at a control volume face. By performing this velocity separation, the pressure at a given node explicitly appears in the discretized form of the continuity equation. As the solution converges, these two calculations approach the same velocity value. Once pressure/velocity coupling is assured on a colocated grid, the modeler has greater flexibility in the choice of solution domain shape and discretization.

3.2.6 Solution of Equations

The discretized set of equations can be written in the following form [53, 54].

$$A_i^* \varphi_i + \sum_{nb} A_{nb}^* \varphi_{nb} = S_\varphi \quad (3.70)$$

where A_i^* is the coefficient for node i , and the subscript nb represents points neighbouring i . For the momentum equation, A_i^* has units of kg/s .

The residual at each point i is calculated as the difference between the left-hand and right-hand sides of Equation (3.70).

$$R_i = A_i^* \varphi_i + \sum_{nb} A_{nb}^* \varphi_{nb} - S_\varphi \quad (3.71)$$

Overrelaxation is used to speed solution convergence. Given current time step value φ_i and previous time step value φ_i^0 ,

$$A_i^* \left(1 + \frac{1}{E}\right) \varphi_i + \sum_{nb} A_{nb}^* \varphi_{nb} = S_\varphi + \frac{A_i^*}{E} \varphi_i^0 \quad (3.72)$$

The variable E has the interpretation of a multiplication factor to the local reference time interval, Δt_i^* , where:

$$\Delta t_i^* = \frac{\rho V_i}{A_i^*} \quad (3.73)$$

and V_i is the volume of control volume i . At each control volume ω_i , the calculation time step Δt is set equal to $E \Delta t_i^*$. For implicit schemes, E can be greater than 1, which

speeds convergence [55]. Values of 10 or greater are possible. As E is constant through the domain but Δt_i^* varies, φ_i advances non-uniformly through the domain. That is, the transient is “distorted.” Therefore this overrelaxation can only be used to aid convergence of steady-state schemes.

The complete set of discrete algebraic equations are solved using a line solver based on the Gauss-Seidel (G-S) solver [53]. A property of G-S solvers is that high-frequency error components are eliminated faster than low-frequency components. This is shown in detail in Appendix D. Given this property, it would be beneficial to solver efficiency if error components could be as high frequency as possible. Multigridging accomplishes this by translating the errors in a given solution iteration onto a coarser grid thereby effectively increasing the frequency of the error component. The advantage of using a multigrid solver is that residuals are reduced much faster per fine grid iteration than by using a single grid alone [54].

Appendix E provides a detailed description of the governing equations and process associated with solving by multigrid. As explained in the Appendix, the code utilizes an additive correction multigrid (ACM) method which sums the flux imbalances over progressively coarser blocks of control volumes and equates the sum to zero. In addition, a ‘W-cycle’ coarsening/refining process is utilized.

3.3 Summary

The mathematical model consists of time-averaged forms of the conservation equations for mass, momentum, and energy. The process of time averaging the momentum and energy equations creates additional averaged turbulent fluctuation terms. These terms are modeled using an eddy viscosity model which assumes, in the case of momentum, a linear relationship between the fluid velocity gradient and the averaged turbulent fluctuation terms. The eddy viscosity model for the averaged turbulent fluctuation terms in the energy equation use a temperature gradient rather than a velocity gradient.

The turbulent eddy viscosity is modeled as a function of turbulent kinetic energy and dissipation rate fields. Transport equations for these fields are solved.

The conservation and transport equations are solved on a discretized domain by integrating the differential equations over discrete control volumes. Flux terms are solved at integration points which ensures a strongly conservative solution. The weak coupling between pressure and velocity is treated by splitting the numerical evaluation of velocity into mass-flow and momentum-flow terms. This allows the use of colocated, as opposed to staggered, grids.

A Gauss-Seidel solver is used which has the property that high-frequency error components are eliminated faster than low-frequency components. To take advantage of this property, multigridging, where flux imbalances are solved on progressively coarser grids, is used.

Chapter 4

Preliminary Validation Studies

4.1 Overview

The role of preliminary validation is to demonstrate that the fundamental mathematical models and numerical solution provide physically justifiable results and to assess the capability of the code to reproduce these results.

The preliminary validation consists of the simulation of five simple problems. The selection of problems represents a logical progression in the complexity of the required physical models and numerical solution. This progression will culminate in the final validation studies provided in the next chapter. The five problems are:

1. laminar flow in a circular pipe;
2. laminar flow in a heated circular pipe;
3. turbulent flow in a circular pipe;
4. turbulent flow in a heated circular pipe; and
5. buoyancy-driven natural convection in a square cavity.

The adequacy of the code in modeling three physical phenomena will be assessed. Specifically, these phenomena are wall shear/pressure drop, heat transfer, and turbulence. Each of these phenomena are found in the more complicated problem of turbulent interchange mixing of coolant in rod bundles. Table 4.1 provides an overview of which phenomena are examined in each of the five preliminary validation cases.

Table 4.1: Phenomena Studied in Preliminary Validation

phenomenon examined	Validation Case				
	laminar pipe flow	laminar pipe flow with heat	turbulent pipe flow	turbulent pipe flow with heat	natural convection
wall shear	•	•	•	•	
heat transfer		•		•	•
turbulence			•	•	

4.2 Laminar Flow in a Circular Pipe

4.2.1 Description of Problem and Analytical Solution

Using laminar flow in a circular pipe as the first validation study is advantageous because the problem is relatively simple and exact solutions for the velocity field and wall shear are available. Code predictions can be compared against these exact solutions in order to determine the correctness and adequacy of the mathematical models and numerical solution.

The problem consists of a circular pipe of radius R and length L . Steady fluid flow through the pipe is allowed to fully develop. The fluid is considered fully developed when there is no axial change in the fluid velocity. The expression for axial velocity, U , as a function of radius is given by the following [2].

$$U(r) = -\frac{\Delta P}{4l\mu} (R^2 - r^2) \quad (4.1)$$

The length l is the distance over which the pressure change ΔP is measured.

The use of an uppercase U suggests time-averaged values (as discussed in Chapter 3). For laminar flow there are no turbulent fluctuations, u' , thus the instantaneous and time-averaged velocities are identical. Either $\bar{u}$ or U could be used in laminar situations without loss of generality.

Integration of the Equation (4.1) over the radius yields an expression for the volumetric flow rate, Q .

$$Q = -\frac{\Delta P \pi R^4}{8l\mu} \quad (4.2)$$

In this validation study, however, bulk velocity, U_b , is used as the inlet boundary condition rather than volumetric flow rate, Q . Given that for a circular pipe $Q = U_b \pi R^2$,

Figure 4.1: Quarter Butterfly Grid used for Laminar Pipe Flow

an expression for the pressure gradient as a function of the inlet bulk velocity is obtained.

$$\frac{\Delta P}{l} = -\frac{8\mu U_b}{R^2} \quad (4.3)$$

Substituting Equation (4.3) into Equation (4.1) yields an expression for $U(r)$ in terms of inlet quantities.

$$U(r) = 2U_b \left(1 - \frac{r^2}{R^2}\right) \quad (4.4)$$

4.2.2 Boundary Conditions and Simulation Details

The domain was discretized using quarter-pipe symmetry. This allowed the use of a “quarter butterfly” mesh, as illustrated in Figure 4.1. The quarter butterfly mesh consists of three structured meshes: a somewhat square ‘core’ and two arc-shaped ‘wings’. This topology removes the problems of skewed control volumes normally seen with structured mesh discretization of pipe sections. Also, the butterfly topology in Figure 4.1 provides good control of domain resolution near the wall.

The mesh consisted of 20 x 20 or 400 nodes in each cross section, with 75 nodes axially, for a total of 30,000 nodes. This corresponds to 26,714 control volumes. In order to observe the trends exhibited by mesh refinement, a second mesh of 25 x 25 or 625 nodes in each cross section was prepared.

As summarized in Table 4.2, four cases were executed. Also presented in the table are the pipe and fluid properties used. The properties roughly correspond to water at 300K. As seen in Table 4.2, the pipe is 25 hydraulic diameters in length.

Table 4.2: Boundary Conditions and Fluid Properties for Laminar Flow in a Circular Pipe

parameter	Case				Units
	1	2	3	4	
Reynolds number, Re	100	200	1000	2000	
bulk velocity, U_b	0.005	0.01	0.05	0.1	$[m/s]$
pipe radius, R	0.01				$[m]$
pipe length, L	0.5				$[m]$
fluid density, ρ	1×10^3				$[kg/m^3]$
fluid viscosity, μ	1×10^{-3}				$[Pa \cdot s]$

The inlet boundary condition consisted of a uniform velocity profile equal to the bulk velocity. Symmetry boundary conditions were applied to the ‘sides’ of the mesh, while a no-slip condition was specified for the pipe wall.

The outlet boundary condition was a reference pressure of zero specified at a single control volume face. Imposing a uniform reference pressure across the outlet could yield poor physical results as a uniform reference pressure would force fully developed conditions at the outlet. Since a uniform inlet velocity is used, the solution requires an appropriate pipe length to develop, and 25 hydraulic diameters may not be sufficient. Using a reference pressure at a single control volume as the outlet condition will not force fully developed conditions at the outlet but rather allow the flow to develop on its own accord.

For higher Reynolds numbers (*i.e.* > 200), it was expected that 25 hydraulic diameters would be insufficient to fully develop the flow. In order to increase the pipe development length, ‘outlet rewinding’ was used. This consists of using the converged outlet velocity profile as the inlet condition for a subsequent full execution of the code. The second code execution effectively simulates 25 hydraulic diameters of pipe length downstream of the first 25 hydraulic diameters of length. Outlet rewinding continues until the flow is observed to be fully developed.

The flow was considered fully developed when the pressure gradient was observed to be constant to within 0.1%. When this criterion was reached, both U and the pressure across the pipe-cross section were observed to be constant. These phenomena are all consistent with fully developed conditions.

The convergence criteria for each code run consisted of a residual of 10^{-4} or less at all points for each of the three momentum equations and pressure equation. As discussed in Chapter 3, Section 3.2.6, the residual is the difference between the left- and right-hand

Table 4.3: Length Required for Development of Laminar Flow

	Case			
	1	2	3	4
Reynolds number	100	200	1000	2000
hydraulic diameters	14	23	74	124

sides of the discretized governing equations.

The code's standard relaxation and multigriding parameters were used.

4.2.3 Analysis of Results

Table 4.3 provides the number of hydraulic diameters of pipe length required to observe fully developed conditions. These values are approximate (to within a few diameters for lower Reynolds numbers and a few tens of diameters for higher) as fully developed conditions occur gradually, rather than suddenly or sharply. As the Reynolds number increases, more hydraulic diameters of development length were required. Since the simulation domain was 25 hydraulic diameters in length, Cases 3 and 4 required two and four 'outlet rewinds', respectively.

Conservation of mass was checked by area-averaging U for each control volume at the outlet. The result for each case was equal to the inlet bulk velocity, U_b .

Figure 4.2 provides a graph of the error, or difference between Equation (4.4) and the code predictions at the fully-developed length as a function of radial distance from the pipe centreline. All of the results were obtained with a $20 \times 20 \times 75$ mesh, with the exception of the 'finer mesh' result, which was obtained using $25 \times 25 \times 75$ mesh.

As shown Figure 4.2, the error increases with increasing Reynolds number, with the largest errors of 3.5% observed near the wall for the $Re = 2000$ case. At the pipe wall ($r = 0.01\ m$), the error for all cases is zero, as the code predicted axial velocity equals the expected value of zero.

Also shown in Figure 4.2 is the influence of increasing the mesh resolution. For the $Re = 2000$ case, increasing the number of nodes by 56% from 400 to 625 per cross section decreases the maximum error from 3.5% to 2.0%. It is expected that increasing the mesh resolution further would improve the results further. Since the maximum errors are observed close to the wall, increasing the nodal resolution in this region is also expected to improve the results. The near-wall region is where the maximum radial gradients in axial velocity are both expected and observed.

Figure 4.2: Error in Prediction of Laminar Axial Velocity, $U(r)$

Table 4.4: Analytical and Predicted Pressure Gradient for Laminar Flow in a Circular Pipe

Re	U_b [m/s]	Nodes in Cross- section	Pressure Gradient		
			Equation (4.3) [Pa/m]	Code Prediction [Pa/m]	Error [%]
100	0.005	400	0.40	0.40032	0.08
200	0.01	400	0.80	0.80067	0.08
1000	0.05	400	4.00	4.0264	0.66
2000	0.1	400	8.00	8.2097	2.62
2000	0.1	625	8.00	8.0927	1.16

Table 4.4 compares the pressure gradient predicted by the code to Equation (4.3). As with the radial distribution of axial velocity, the error in the pressure gradient increases with Reynolds number. This is attributed to the higher velocity gradients in the near-wall region. Increasing the number of nodes in the cross section is again observed to improve the results.

This first validation study confirms the code's ability to conserve mass and recreate physically justifiable velocity profiles and pressure gradients. The pressure gradient results suggest momentum is properly conserved. Sensitivity to the number of mesh nodes was observed, with better results obtained from finer meshes.

4.3 Laminar Heat Transfer in a Circular Pipe

4.3.1 Description of Problem and Analytical Solution

In order to study the code's ability to model heat transfer from walls and through the fluid, the problem of laminar flow through a pipe was revisited with the addition of heated walls.

The problem investigated consisted of an unheated length of pipe followed by a section with heated walls. The unheated length enables the flow to reach fully-developed conditions prior to the application of heat. This is referred to as a 'thermal entry length' type problem [47].

Two types of heated wall were investigated: constant temperature and constant heat flux.

The Nusselt number, Nu , is a dimensionless measure of heat transfer, defined in terms of the wall heat transfer coefficient, h_w , pipe hydraulic diameter, D_h , and fluid thermal conductivity, Γ . The wall heat transfer coefficient, h_w , can be written in terms of the wall heat flux, q_w'' , and the difference between the wall and bulk fluid temperatures, $T_w - T_b$.

$$\begin{aligned} Nu &= \frac{h_w D_h}{\Gamma} \\ &= \frac{q_w'' D_h}{(T_w - T_b) \Gamma} \end{aligned} \quad (4.5)$$

The bulk temperature, T_b is defined as the temperature which, when multiplied by the mass flow rate and fluid heat capacity, yields the axial energy transport rate [47]. It can also be defined as the mass flow rate weighted temperature.

Solution of the energy equation with constant temperature walls and a fully-developed velocity field yields a constant Nu value of 3.66 once the thermal field is fully devel-

oped [47]. For constant heat flux walls, Nu equals 48 elevenths (or 4.364) once the thermal field is fully developed [56].

Incropera and De Witt [47] present a correlation attributed to Hausen which provides a length-averaged Nusselt number, $\overline{Nu}_L$, for thermal development of a flow with constant temperature walls and a thermal entry length.

$$\overline{Nu}_L(x) = 3.66 + \frac{0.0668(D/x)\text{RePr}}{1 + 0.04[(D/x)\text{RePr}]^{2/3}} \quad (4.6)$$

Note that as $x \rightarrow \infty$, the average Nusselt number approaches 3.66. Given the definition of length-averaged Nusselt number,

$$\overline{Nu}_L(x) = \frac{1}{x} \int_0^x Nu(\eta) d\eta \quad (4.7)$$

where η is a dummy variable, Equation (4.6) can be rewritten as a local Nusselt number, Nu .

$$\begin{aligned} Nu(x) &= \frac{d}{dx} (x \overline{Nu}_L(x)) \\ Nu(x) &= \frac{d}{dx} \left\{ 3.66x + x \frac{0.0668(D/x)\text{RePr}}{1 + 0.04[(D/x)\text{RePr}]^{2/3}} \right\} \\ &= 3.66 + 0.00178 [(D/x)\text{RePr}]^{5/3} \left\{ 1 + 0.04 [(D/x)\text{RePr}]^{2/3} \right\}^{-2} \end{aligned} \quad (4.8)$$

The Graetz number, Gz , is defined as the Reynolds number times Prandtl divided by x/D .

$$Gz = \frac{\text{RePr}}{x/D} \quad (4.9)$$

The Graetz number measures the ratio of bulk heat transfer to conductive heat transfer as a function of hydraulic diameters of length from the start of the heated section of pipe. Hausen's expression is therefore written as follows.

$$Nu = 3.66 + 0.00178 Gz^{5/3} \left\{ 1 + 0.04 Gz^{2/3} \right\}^{-2} \quad (4.10)$$

Equation (4.10) can be compared to the code-predicted average Nusselt number as the thermal field develops for the case of constant temperature walls and a thermal entry length.

4.3.2 Boundary Conditions and Simulation Details

The results of the previous study of laminar flow in an unheated pipe were used to provide fully developed inlet velocity and pressure fields. A fully developed inlet is a necessary condition for thermal entry length type problems.

Table 4.5: Thermal Properties for Laminar Flow in Heated Pipe

parameter	Case		units
	const T wall	const q'' wall	
wall temperature, T_w	400		[K]
wall heat flux, q''_w		10^5	[W/m ²]
bulk velocity, U_b	0.01		[m/s]
heat capacity, c_p	10^3		[J/kg · K]
thermal conductivity, Γ	1.0		[W/m · K]
Prandtl number, Pr	1.0		

The pipe dimensions were the same as used in the previous section, as given in Table 4.2. The fluid thermal properties for the constant wall temperature and constant wall heat flux problems are summarized in Table 4.5.

The meshes for the heat transfer study were the same as the previous unheated flow study: quarter-pipe butterfly meshes of 20 x 20 or 400 cross-sectional nodes and 75 axial nodes for a total of 30,000 nodes (Figure 4.1).

The boundary conditions were the same as the previous study with the exception of the specification of either constant temperature or constant heat flux walls.

The convergence criteria for U , V , and W was the same as for the laminar flow in an unheated pipe cases. The convergence criterion for the energy equation was a solution residual of 10^{-4} or less at all nodes.

4.3.3 Analysis of Results

The bulk temperature, T_b , at each cross-section x_i is calculated by mass flow rate weighting the local fluid temperature and integrating over the pipe radius.

$$T_b(x_i) = \frac{1}{\rho U_b \pi R^2} \int_0^R \rho U(x_i, r) c_p T(x_i, r) 2\pi r dr \quad (4.11)$$

The wall heat flux, q''_w , for the case of constant temperature walls is determined by calculating the change in heat flow between cross sections x_i and x_{i+1} .

$$q''_w = \frac{c_p \rho U_b R [T_b(x_{i+1}) - T_b(x_i)]}{2(x_{i+1} - x_i)} \quad (4.12)$$

This assumes the grid is of uniform thickness in the x direction, which is the case in this investigation.

Figure 4.3: Nusselt Numbers for Laminar Flow in a Heated Pipe

Using the previous two equations in conjunction with the definition of the Nusselt number, Equation (4.5), the Nusselt number predicted by the code as a function of x_i was calculated. Figure 4.3 illustrates the code predicted Nusselt number versus the inverse of Graetz number. A value of $Gz^{-1} = 0$ corresponds to the start of the heated section of pipe.

As shown in Figure 4.3, the constant wall temperature and constant wall heat flux simulations both approach the theoretical Nu values of 3.66 and 4.364, respectively. From $Gz^{-1} = 0.08$ to 0.12 the average of the predicted Nusselt values is 3.654 for the constant wall temperature case and 4.368 for the constant wall heat flux case. This represents errors of -0.16% and 0.09%, respectively.

Figure 4.3 shows the predicted local Nusselt number follows the trend given by the differentiation of Hausen's relation given by Equation (4.10). A maximum difference of 11.7% occurs near the start of the heated section of pipe at an inverse Graetz number of $Gz^{-1} = 0.0084$. After $Gz^{-1} = 0.02$, the maximum error is 2.6%.

Figure 4.3 also shows the effect of changing the Prandtl number. A constant wall heat flux simulation with a Prandtl number of 0.1 was performed by decreasing the heat capacity to $100 \text{ J/kg} \cdot \text{K}$. The predicted local Nusselt numbers follow the same values

exhibited by the $Pr=1.0$ case, as expected. The data points for the $Pr=0.1$ case are spaced further apart because the inverse Graetz number is a function of the Prandtl number. The same point x has a higher value of $1/Gz$ for smaller values of Pr . The axial mesh resolution both cases are identical.

The results of the heated wall problems (both constant temperature and constant heat flux) are physically justifiable. This indicates that the code is correctly predicting heat transfer from the walls into the fluid as well as convection of heat along the pipe. The next step in the validation process is to consider the influence of turbulence.

4.4 Turbulent Flow in a Circular Pipe

4.4.1 Description of Problem and Analytical Solution

By invoking the $k - \epsilon$ eddy viscosity turbulence model, predictions involving turbulence were investigated. The problem investigated consisted of a smooth, circular pipe with a steady fluid flow, much like the laminar flow problem given in Section 4.2.1.

The code-predicted velocity and turbulence fields were compared to experimentally-obtained expressions for Fanning friction factor, f , radial profile of time-averaged axial velocity, U , and turbulence intensity, T_u .

In order to calculate the Fanning friction factor, the shear stress at the wall must be determined. In a Newtonian fluid, the shear stress parallel to the pipe's axis, τ , is related to the radial gradient of the axial velocity with the constant of proportionality defined as the dynamic molecular viscosity, μ .

$$\tau = -\mu \frac{\partial U}{\partial r} \quad (4.13)$$

By performing a force balance on the fluid in the pipe, the shear stress at the wall, τ_w , can be related to the pressure gradient, $\Delta p/l$.

$$\tau_w = -\frac{\Delta p}{l} \frac{R}{2} \quad (4.14)$$

The Fanning friction factor, f , can be expressed in terms of the wall shear¹.

$$f = \frac{2\tau_w}{\rho U_b^2} \quad (4.15)$$

¹Some references use f to represent the D'Arcy friction factor, which is exactly four times larger than the Fanning factor. The symbol λ is used to represent the D'Arcy factor in this thesis, thus $\lambda = 4f$. This thesis uses the Fanning factor unless clearly stated otherwise.

Substituting Equation (4.14) into Equation (4.15) provides an expression for determining the friction factor, f , based upon a predicted pressure gradient.

$$f = -\frac{\Delta p}{l} \frac{R}{\rho U_b^2} \quad (4.16)$$

Colebrook [9] provides an expression for f based upon Moody's diagram for the turbulent friction factor in circular pipes (Equation (2.9) in Chapter 2). Blasius (referenced in Schlichting [13]) also provides an expression for the friction factor.

$$f = 0.0791 \text{Re}^{-0.25} \quad (4.17)$$

By using Equation (4.16) with the pressure gradient predicted by the code, a code-predicted friction factor can be compared to Colebrook's and Blasius's expressions.

The radial profile of axial velocity is 'blunted' or flatter for turbulent flows as compared to laminar flows (*e.g.* Equation (4.1)). Schlichting [13] references Nikuradse's expression for the radial profile of axial velocity based on boundary layer theory and experimental observation.

$$U(r) = U_b \frac{(n+1)(2n+1)}{2n^2} \left(\frac{r}{R} \right)^{\frac{1}{n}} \quad (4.18)$$

The constant n is determined empirically, and ranges from 6.0 for a Reynolds number of 4×10^3 , to 7.0 for $\text{Re} = 1.1 \times 10^5$, to as high as 10 for $\text{Re} = 3.2 \times 10^6$. One non-physical aspect of Equation (4.18) is a non-zero slope at the pipe centreline. It is therefore expected the code and Equation (4.18) will be somewhat different in the region of the centreline.

The turbulence intensity is calculated by rearranging Equation (3.54) in Section 3.1.8.

$$T_u = \frac{1}{U_b} \sqrt{\frac{2}{3}k} \quad (4.19)$$

4.4.2 Boundary Conditions and Simulation Details

As with the laminar flow investigations, a quarter-butterfly mesh was used (Figure 4.1). Because higher Reynolds numbers were used in the turbulent study, the pipe length was doubled to 50 hydraulic diameters and the number of axial nodes doubled to 150.

The pipe dimensions and fluid properties are provided in Table 4.6.

The use of a turbulence model requires a few additional boundary conditions. First, inlet turbulence intensity and length scales are required. The values given in Table 4.6 were chosen based on trial executions of the code. Regardless of the choice of inlet intensity and length scale, the eventual exit turbulent field length scale and intensity

Table 4.6: Boundary Conditions and Fluid Properties for Turbulent Flow in a Circular Pipe

parameter	Case				Units
	1	2	3	4	
Reynolds number, Re	10,000	11,513	23,973	100,000	
bulk velocity, U_b	0.50	0.5756	1.199	5.0	$[m/s]$
pipe radius, R	0.01				$[m]$
pipe length, L	1.0				$[m]$
fluid density, ρ	10^3				$[kg/m^3]$
fluid viscosity, μ	10^{-3}				$[Pa \cdot s]$
inlet turb. intensity, T_u	5%				
inlet length scale, L_ϵ	0.01				$[m]$
near-wall node location, y^+	50				

approached similar values. The values given in Table 4.6 are close to the eventual outlet values, thus these values develop the turbulence field faster than other values.

Another requirement of turbulent flow simulations is the careful placement of the near wall nodes in order to properly use the law of the wall as momentum and turbulence equation boundary conditions. This was accomplished by using the definition of y^+ to estimate y , the required distance from the near-wall nodes to the wall.

$$y = \frac{2Ry^+}{Re} \sqrt{\frac{2}{f}} \quad (4.20)$$

The friction factor, f , for a given Reynolds number is estimated during mesh generation by using Blasius' equation (Equation (4.17)). Both the Reynolds number and f are functions of bulk velocity, thus different inlet velocities require different meshes due to the corresponding change in y .

As with the laminar flow study, outlet rewinding was used to obtain fully developed conditions. A constant pressure gradient (to within 0.1%) was used as the criterion for achievement of fully-developed flow.

Similar to the the previous studies, the convergence criteria consisted of a maximum residual of 10^{-4} or less for the U , V , W , and P equations at all nodes.

4.4.3 Analysis of Results

Figure 4.4 compares the code-predicted Fanning friction factors with those given by Colebrook's and Blasius' expressions. Also shown in Figure 4.4 is the friction factor

Figure 4.4: Friction Factors for Turbulent Flow in a Pipe

obtained from the velocity profile of Tsuji and Morikawa's laser-doppler anemometry measurements of turbulent flow in a circular pipe [57].

From Figure 4.4 it is apparent that the code overpredicts both the Colebrook and Blasius friction factors. The code predicted values of f are between 6.2% and 7.8% higher than Colebrook's expression and 3.5% and 8.8% higher than Blasius'. The code prediction at a Reynolds number of 11,513 is 5.8% lower than that obtained from analysis of Tsuji and Morikawa's velocity profile data.

Linear regression of the code predictions yields a curve fit of the form $f = 0.0713\text{Re}^{-0.234}$, as compared to Colebrook's $f = 0.06646\text{Re}^{-0.234}$ and Blasius' $f = 0.0791\text{Re}^{-0.25}$. The coefficients of determination for the fits are 0.997, 0.999, and 1.000, respectively. A value of 1 indicates a perfect logarithmic curve fit, hence the code prediction follows the logarithmic form closely. The dependence of friction on Reynolds number predicted by the code is virtually identical to Colebrook's expression and only slightly weaker than given by Blasius.

The axial velocity radial profiles predicted for $\text{Re}=10,000$ and $\text{Re}=11,513$, normalized to bulk velocity, are provided in Figure 4.5. Included are Tsuji and Morikawa's [57] measured values for turbulent pipe flow ($\text{Re}=11,513$) and Nikuradse's expression (Equa-

Figure 4.5: Radial Profile of Turbulent Axial Velocity

tion (4.18)) using $n = 6$ and $n = 7$. The value $n = 6$ corresponds to a Reynolds number of approximately 10,000 and $n = 7$ to $Re=110,000$.

Unfortunately, Tsuji and Morikawa do not provide error information. Error bars were added to their data to illustrate the magnitude of a hypothetical $\pm 2\%$ error in their measurement.

The predicted velocity profile is noticeably ‘flatter’ in the centre of the pipe than either the Tsuji and Morikawa data or Nikuradse’s expression. This is consistent with the observed overprediction in friction factor as higher wall friction will steepen the profile close to the wall, thereby flattening the middle of the profile in order to meet continuity. The maximum error between Tsuji and Morikawa and the code predicted profile (for $Re=11,513$) is 5.2% and located near the pipe wall.

Figure 4.6 compares the predicted radial turbulence intensity, T_u , against the measured values of Tsuji and Morikawa [57] for a Reynolds number of 29,973. As with their axial velocity data, Tsuji and Morikawa do not provide error data. Error bars were added to illustrate the magnitude of a hypothetical $\pm 1\%$ change in turbulence intensity.

As seen in Figure 4.6, the code overpredicts T_u by 0.5% in the centre of the pipe while underpredicting T_u by 1.2% near the wall.

Figure 4.6: Radial Profile of Axial Turbulent Intensity

The friction factor is directly related to the near-wall turbulent kinetic energy since:

$$\begin{aligned}
 f &= \frac{2\tau_w}{\rho U_b^2} \\
 &= \frac{2\sqrt{c_\mu}k}{U_b^2}
 \end{aligned} \tag{4.21}$$

Figure 4.4 indicates that the code overpredicts Colebrook's and Blasius' friction factor correlations, but underpredicts the friction factor obtained from Tsuji and Morikawa's velocity profile. Thus, the code appears to underpredict the near-wall turbulent kinetic energy, k , as compared to Tsuji and Morikawa, but overpredicts k as compared to Colebrook and Blasius. Further, Figure 4.6 indicates that the code underpredicts the near-wall turbulence intensity as measured by Tsuji and Morikawa. This is consistent with the observation that the code underpredicts the Tsuji and Morikawa near-wall turbulent kinetic energy based on the friction factors.

In summary, the turbulent kinetic energy and dissipation fields are calculated accurately enough to predict turbulent friction factors to within 8% as compared to published correlations and within 5.2% as compared to experimental data. Further, the turbulence intensity is predicted to within a few percent of experimental results. Observed differences between calculated and experimental friction factors and turbulence intensity are

consistent because both results suggest an underprediction of turbulent kinetic energy near the pipe wall.

4.5 Turbulent Heat Transfer in a Circular Pipe

4.5.1 Description of Problem and Analytical Solution

The code's ability to model turbulent heat transfer can be investigated by the addition of heated walls to the previous section's turbulent pipe flow problem. Similar to the laminar heat transfer problem investigated in Section 4.3, a 'thermal entry' type problem is explored in which a fully developed, unheated flow is exposed to heated pipe walls.

Unlike the case of laminar flow, however, the turbulent heat transfer problem does not provide a straightforward solution of the energy equation. Some expressions are available for the case of constant wall heat flux, thus constant wall heat flux will be used as a boundary condition in this investigation.

Given a wall temperature T_w , and wall heat transfer, q_w'' , Mills [56] introduces a non-dimensional temperature, T^+ .

$$T^+ = \frac{(T_w - T)\rho c_p u_\tau}{q_w''} \quad (4.22)$$

Mills provides an expression for the non-dimensional centreline temperature, T_c^+ , based on integration of the temperature law of the wall.

$$T_c^+ = 5\text{Pr} + 5 \ln(5\text{Pr} + 1) + 2.25 \left\{ \ln \left[\frac{\text{Re}}{60} \sqrt{\frac{f}{2}} \right] - 1 \right\} \quad (4.23)$$

Based on the definition of the Nusselt number, Mills provides the following analytical expression.

$$\text{Nu} = \text{RePr} \sqrt{\frac{f}{2}} \left[\left(\frac{T_w - T_b}{T_w - T_c} \right) T_c^+ \right]^{-1} \quad (4.24)$$

The ratio $(T_w - T_b)/(T_w - T_c)$ is a function of Reynolds number and Prandtl number, as given in Table 4.7. Mills [56] comments that Equation (4.24) agrees well with experiment for $\text{Re} > 10^4$ and $0.5 < \text{Pr} < 30$.

4.5.2 Boundary Conditions and Simulation Details

As with the laminar heat transfer in a circular pipe, the results of the unheated simulations were used to provide a fully developed inlet condition for the heat transfer study.

Table 4.7: Turbulent Heat Transfer Ratio $(T_w - T_b)/(T_w - T_c)$ from Mills [56]

Re	Pr				
	10^{-2}	10^{-1}	1	10	10^2
10^4	0.589	0.692	0.865	0.958	0.992
10^5	0.639	0.761	0.877	0.962	0.993

Table 4.8: Turbulent Heat Transfer in a Circular Pipe Boundary Conditions

parameter	Case							units
	1	2	3	4	5	6	7	
Re	10^4				1.1×10^4	10^5		
Pr	0.1	1.0	10	100	1.0	0.01	0.1	
q_w''	10^5							$[W/m^2]$

Seven cases were investigated using different Reynolds and Prandtl numbers, as summarized in Table 4.8.

The mesh was the same as that used in the turbulent pipe flow study: a quarter-pipe butterfly mesh with 400 nodes per cross-section and 150 axial nodes.

The convergence criteria was the same as previous studies: a residual at every node of 10^{-4} or less for each of U, V, W, P, and energy equations.

4.5.3 Analysis of Results

The Nusselt numbers for the seven cases were calculated the same as for the laminar heat transfer problem by using Equations (4.5) and (4.11) in Section 4.3.

The code predicted Nusselt numbers are compared to Equation (4.24) in Table 4.9. A wide range of error values were observed, with the lowest errors occurring for the two cases with Prandtl numbers of unity. The highest error was yielded by Case 7. Equation (4.24) is not used for Case 4 as the Prandtl number exceeds the range of applicability.

Also provided in Table 4.9 is a comparison of code predicted values of $(T_w - T_b)/(T_w - T_c)$ with that published by Mills [56]. While the differences in Nusselt numbers ranged considerably, a much closer agreement was observed in the predicted and published values of $(T_w - T_b)/(T_w - T_c)$.

An interesting aspect of the results in Table 4.9 is that Cases 2 and 5, which yielded the smallest difference between predicted Nu and Equation (4.24) did not provide the smallest difference in the temperature ratio. Mills obtains Equation (4.24) by assuming

Table 4.9: Predicted Turbulent Heat Transfer in Circular Pipe

Case	Re	Pr	Nusselt, Nu			$(T_w - T_b)/(T_w - T_c)$		
			Predicted Value	Equation (4.24)	Error %	Predicted Value	Table 4.7	Error %
1	10^4	0.1	12.69	16.22	-0.22	0.692	0.678	1.48
2		1.0	42.34	42.21	-0.3	0.822	0.865	-4.96
3		10	114.3	89.27	28.0	0.986	0.992	-0.55
4		100	255.4	n/a	n/a	0.943	0.958	-1.61
5	1.1×10^4	1.0	46.67	46.95	-0.6	0.825	0.865	-4.62
6	10^5	0.01	52.73	61.64	14.5	0.778	0.761	2.25
7		0.1	13.51	9.42	43.4	0.643	0.639	0.69

the following near-wall relationship between turbulent eddy viscosity and dimensionless distance from the wall:

$$\mu_t = \mu \left(\frac{2}{5} y^+ - 1 \right) \quad y^+ > 30 \quad (4.25)$$

The code, on the other hand, solves transport equations for k and ε in order to obtain the near-wall turbulent eddy viscosity. For comparison, Equation (4.25) predicts a μ_t value of $0.0198 \text{ Pa} \cdot \text{s}$ at $y^+ = 52$ for Case 2 while the code predicts $0.0138 \text{ Pa} \cdot \text{s}$ at the same location, a difference of 30%. Thus the μ_t -based relationship between Nu and $(T_w - T_b)/(T_w - T_c)$ assumed in Equation (4.24) is not the same as predicted by the code. Further, Mills states that the temperature ratio is “relatively insensitive” to choice of near-wall profile. Hence, the good Nusselt number agreement for Cases 2 and 5 may be fortuitous, while the poorer temperature ratio agreement is likely a more accurate reflection of the accuracy of the near-wall heat transfer.

4.6 Laminar Buoyancy-Driven Convection in a Square Cavity

4.6.1 Description of Problem and Benchmark Solution

Buoyancy-driven flow in a square cavity combines momentum, buoyancy, and heat transfer models. Predictions of laminar buoyancy-driven flow were obtained and compared to the published benchmarks.

The domain for the buoyancy driven flow problem is illustrated in Figure 4.7. A square cavity of length L on each side is held at a hot temperature, T_h , on the left

Figure 4.7: Domain for Buoyancy Driven Flow in a Square Cavity

side and a cold temperature, T_c , on the right. The top and bottom walls are adiabatic. Gravity acts in the downward direction.

An important dimensionless quantity for buoyancy driven heat transfer is the Rayleigh number, Ra , defined as the Grashof number multiplied by the Prandtl number.

$$\begin{aligned}
 Ra &= GrPr \\
 &= \left[\frac{g\beta (T_h - T_c) L^3}{\nu^2} \right] \left[\frac{\nu}{\alpha} \right] \\
 &= \frac{g\beta (T_h - T_c) L^3}{\nu\alpha}
 \end{aligned} \tag{4.26}$$

The Rayleigh number represents the ratio of buoyancy-driven convection of heat to conduction. Larger values of Ra indicate greater buoyancy-driven convection.

The numerical benchmark solutions of de Vahl Davis [58] and Hortmann and Perić [54] were compared to the code results. While de Vahl Davis provides results for $Ra=10^3$, 10^4 , and 10^5 , Hortmann and Perić provide results for $Ra=10^4$ and 10^5 . Hortmann and Perić report their results are accurate to within 0.01% while de Vahl Davis reports an error range of 0.1% for $Ra=10^3$ and 1% for $Ra=10^5$. Both references claim grid independent results.

Five parameters were chosen for comparison with de Vahl Davis and Hortmann and Perić. These parameters are:

1. maximum velocity in x-direction, U_{max} ;
2. maximum velocity in z-direction, W_{max} ;
3. average Nusselt number in x-direction, $\overline{Nu}_x$;
4. midplane Nusselt number in x-direction, $Nu_{x=1/2}$; and

Table 4.10: Buoyancy Conditions for Buoyancy-Driven Flow in a Square Cavity

Parameter	Case			Units
	1	2	3	
Rayleigh number, Ra	10^3	10^4	10^5	
hot wall temp, T_{hot}	310.921	409.21	400.	$[K]$
cold wall temp, T_{cold}	300			$[K]$
cavity length, L	1×10^{-2}		2.2195×10^{-2}	$[m]$
density, ρ	1.1614			$[kg/m^3]$
heat capacity, c_p	1.007×10^3			$[J/kg \cdot K]$
dynamic viscosity, μ	184.6×10^{-7}			$[Pa \cdot s]$
kinematic viscosity, ν	15.89×10^{-6}			$[m^2/s]$
thermal conductivity, k	26.3×10^{-3}			$[W/m \cdot K]$
thermal diffusivity, α	22.5×10^{-6}			$[m^2/s]$
thermal expansion, β	3.333×10^{-2}			$[K^{-1}]$
Prandtl number, Pr	0.707			
gravity, g	9.81			$[m/s^2]$

5. hot-wall Nusselt number in x-direction, $Nu_{x=0}$.

Hortmann and Perić do not provide results for parameters 4 and 5, however.

4.6.2 Boundary Conditions and Simulations Details

Three different Rayleigh numbers were investigated: 10^3 , 10^4 , and 10^5 . These were obtained by varying the temperature of the hot wall. Table 4.10 provides a summary of the fluid and cavity properties. The working fluid was air.

The mesh was designed to simulate a two-dimensional problem. Four uniform grids were generated with 11×11 , 21×21 , 41×41 and 81×81 nodes in the vertical and horizontal directions. Thus, the number of control volumes were 10×10 , 20×20 , 40×40 , and 80×80 , respectively. In the front-to-back direction, three nodes, or two control volumes were used.

The boundary conditions consisted of adiabatic walls at the top and bottom ($+z$ and $-z$), with constant temperature walls at the sides ($+x$ and $-x$). The front and back walls ($+y$ and $-y$) were specified using symmetry conditions. This created a two-dimensional system in the x and z directions only. As there is no outlet in this problem, the pressure boundary condition consisted of a specification of a reference pressure of zero at a corner node.

To facilitate comparison of the code predictions with benchmark solutions, the results

were normalized using length, time, velocity, and mass scales. The length scale, L , was the cavity width. The time scale was $t = L^2/\alpha$ (length scale squared divided by the thermal diffusivity). The velocity scale was $U = L/t$, while the mass scale was $m = \rho L^3$.

The temperature was normalized using the following.

$$\theta = \frac{T - T_{cold}}{T_{hot} - T_{cold}} \quad (4.27)$$

Normalized quantities other than temperature are indicated by a caret, (*e.g.* $\hat{U}$, $\hat{x}$).

All code runs used the same target maximum residual at all nodes of 10^{-4} for the U , V , W , P , and energy equations. Although convergence was slower for higher Rayleigh values, all cases converged to within the target residuals.

4.6.3 Analysis of Results

When using non-dimensional quantities, the Nusselt number at horizontal position $\hat{x}$ is given by the following formula [58].

$$\text{Nu}_{\hat{x}} = \int_0^1 \left(\hat{U}\theta - \frac{\partial\theta}{\partial\hat{x}} \right) d\hat{x} \quad (4.28)$$

The average Nusselt number is calculated by integrating $\text{Nu}_{\hat{x}}$ over all values of $\hat{x}$.

$$\overline{\text{Nu}} = \int_0^1 \text{Nu}_{\hat{x}} d\hat{x} \quad (4.29)$$

Tables 4.11 through 4.13 compare the code-predicted monitored values with those of de Vahl Davis and Hortmann and Perić.

For lower Rayleigh number values, code-predicted values were closer to benchmark results than for higher values. In particular, $\hat{U}_{max}$ for $\text{Ra}=10^5$ exhibited the largest difference between code-predicted and benchmark values with an error of 28%, while $\hat{W}_{max}$ differed by 1.6%. This suggests finer mesh resolutions are required for the higher Rayleigh number values. For $\text{Ra}=10^5$, Hortmann and Perić required 641x641 node meshes in order to observe grid independence. De Vahl Davis did not use meshes finer than 81x81 nodes for $\text{Ra}=10^5$ and did not demonstrate grid independence for this Rayleigh number.

The $\text{Ra}=10^5$ case with a 81x81 mesh was re-run using a non-uniform mesh in which near-wall control volumes were refined. There was no appreciable change in the accuracy of the results as compared to the uniform mesh results. This observation was also reported by Hortmann and Perić [54].

Nusselt values compared favourably for all Rayleigh cases. The residual, or difference between the code predictions and benchmark values, increased with the Rayleigh numbers.

Table 4.11: Results for Rayleigh Number of 10^3

Parameter	Grid Size				Ref [58]	Difference (%)
	11x11	21x21	41x41	81x81		
$\hat{U}_{max}$	4.290	3.795	3.683	3.661	3.649	0.33
$\hat{W}_{max}$	4.495	3.855	3.740	3.709	3.697	0.32
Nu	1.191	1.133	1.121	1.119	1.118	0.09
$Nu_{1/2}$	1.181	1.136	1.122	1.119	1.118	0.09
Nu_0	1.174	1.121	1.116	1.115	1.117	-0.18

Table 4.12: Results for Rayleigh Number of 10^4

Parameter	Grid Size				Ref [58]	Ref [54]	Difference (%)
	11x11	21x21	41x41	81x81			
$\hat{U}_{max}$	18.534	16.900	16.406	16.252	16.178	16.176	0.46
$\hat{W}_{max}$	24.309	21.277	19.920	19.747	19.617	19.624	0.66
Nu	2.720	2.419	2.2880	2.255	2.243	2.245	0.54
$Nu_{1/2}$	2.646	2.414	2.289	2.255	2.243	n/a	0.54
Nu_0	2.796	2.400	2.276	2.249	2.238	n/a	0.49

Table 4.13: Results for Rayleigh Number of 10^5

Parameter	Grid Size				Ref [58]	Ref [54]	Difference (%)
	11x11	21x21	41x41	81x81			
$\hat{U}_{max}$	42.807	49.256	45.805	44.419	34.73	34.74	28
$\hat{W}_{max}$	39.063	86.679	73.027	69.692	68.59	68.64	1.6
Nu	3.826	5.484	4.828	4.595	4.519	4.522	1.7
$Nu_{1/2}$	3.612	5.588	4.849	4.595	4.519	n/a	1.7
Nu_0	4.645	5.471	4.787	4.581	4.509	n/a	1.6

Table 4.14: Convergence and Extrapolation Results

Rayleigh Number	Order n	Extrapolated $\overline{Nu}_\infty$	Benchmark $\overline{Nu}$ [58]	Difference (%)
10^3	2.58	1.1186	1.118	0.05
10^4	1.99	2.247	2.243	0.17
10^5	1.60	4.487	4.519	-0.71

Figures 4.8 through 4.10 provide plots of the θ , $\hat{U}$ (horizontal), and $\hat{W}$ (vertical) contours for the three different Rayleigh numbers. As the quantities presented in Figures 4.8 through 4.10 are normalized, each of the 11 contours represent an increment of 10%. These contours compare very favourably with those published by de Vahl Davis.

A benefit of choosing uniform mesh sizes of 11x11, 21x21, 41x41, and 81x81 is that each grid width, $\Delta\hat{x}$, is half that of the previous. This allows the determination the order of convergence of the solution.

By assuming the error between $\overline{Nu}$ for grid size $\Delta\hat{x}$ and the grid independent value $\overline{Nu}_\infty$ is expressible as a power of grid size:

$$\overline{Nu}_{\Delta\hat{x}} - \overline{Nu}_\infty = e^C \Delta\hat{x}^n \quad (4.30)$$

and taking the logarithm of both sides, yields the following.

$$\ln(\overline{Nu}_{\Delta\hat{x}} - \overline{Nu}_\infty) = C + n \ln(\Delta\hat{x}) \quad (4.31)$$

For each Ra value, the error in the solution is a straight line on a log-log plot with slope n and offset C . The constants n and C can be found from the numerical results:

$$n = \frac{\ln(\overline{Nu}_1 - \overline{Nu}_2) - \ln(\overline{Nu}_2 - \overline{Nu}_3)}{\ln(\Delta\hat{x}_1/\Delta\hat{x}_2)} \quad (4.32)$$

Rearrangement of the equations yields an expression for the extrapolated Nusselt number, $\overline{Nu}_\infty$.

$$\overline{Nu}_\infty = \overline{Nu}_3 - \left[\frac{\overline{Nu}_2 - \overline{Nu}_3}{\Delta\hat{x}_1^n - \Delta\hat{x}_2^n} \right] \Delta\hat{x}_3^n \quad (4.33)$$

Figure 4.11 illustrates the logarithmic convergence trend of the average Nusselt number, $\overline{Nu}$. The residual is defined as the difference between the predicted and benchmark $\overline{Nu}$ normalized to the benchmark $\overline{Nu}$. The residuals are higher for larger Rayleigh values.

Table 4.14 summarizes the calculated order-of-convergence, n , extrapolated solution, $\overline{Nu}_\infty$, and the benchmark solution presented by de Vahl Davis [58].

As expected, the 10^3 and 10^4 extrapolations were far more accurate than the 10^5 extrapolation. However, the extrapolated average Nusselt numbers in all three cases

Figure 4.8: Natural Convection Temperature, θ , Contours Figure 4.9: Natural Convection $\hat{U}$ Velocity Contours Figure 4.10: Natural Convection $\hat{W}$ Velocity Contours

Figure 4.11: Logarithmic $\overline{Nu}$ Residual vs. Grid Size for Buoyancy-Driven Flow

yield results more accurate than the non-extrapolated results in Tables 4.11 through 4.13.

The order of convergence for the $Ra=10^3$ cases was in excess of 2. As the Rayleigh number increased, and advection of energy became more important, the order of convergence decreased.

The buoyancy-driven flow study reaffirms the adequacy of the code's laminar mass, momentum, and heat transfer models. The maximum velocity values differed from benchmark values more than did Nusselt numbers. While grid independent values were approached for lower Rayleigh values, converged results for $Ra=10^5$ did not exhibit grid independence after using an 81×81 mesh.

4.7 Summary of Preliminary Validation

The objective of the preliminary validation is to demonstrate that the fundamental mathematical models and numerical schemes provide physically justifiable results.

Laminar flow cases confirmed conservation of mass, momentum, and energy. Sensitivity to grid resolution was observed in the prediction of the axial pressure gradient

and radial velocity profile. Heat transfer from the pipe walls to the laminar flow was predicted very well.

Turbulent flow cases confirmed the $k - \varepsilon$ turbulence model produced physically justifiable results, however overprediction of wall friction suggests an overprediction of turbulent eddy viscosity in the near-wall region. This, combined with other factors, suggests an underprediction of the turbulent dissipation rate, ε , near the wall. Turbulent heat transfer from the pipe walls to the fluid matched published temperature ratios within 5%. Comparison to published Nusselt number correlations yielded an error range of 0.22% to 48% within the correlation's range of applicability.

The natural convection in a square cavity problem redemonstrated the accuracy of code predictions of wall heat transfer for laminar flow as evidenced by comparison with published benchmarks. Results which suggested grid independence were obtained for the $Ra=10^3$ and 10^4 cases. However, finer grids are required for the $Ra=10^5$ case in order to observed grid independent results.

The set of preliminary validation exercises has provided both confidence in the code's fluid modeling ability while revealing areas which require careful attention during the final validation studies. Specifically, the calculation of near-wall values of k and ε should be monitored carefully.

Chapter 5

Final Validation Studies

5.1 Selection of Validation Dataset

A number of candidate datasets were considered for the validation of turbulent interchange mixing. Table F.1 in Appendix F provides a summary of various experiments involving axial flow through rod bundle assemblies. A ranking system was employed to identify datasets which provide the best combination of measurement quality and applicability to the current investigation. The rating system shown in Table F.1 uses a ranking between zero and four stars. Datasets involving spacer grids or rod appendages are rated lower due to the presence of flow-diversion mixing. Datasets involving measurements of wall shear, pressure drop, and thermal mixing are rated higher.

The dataset chosen for the final validation studies is that of Seale [37]. Seale's dataset is advantageous for a number of reasons:

1. the flow is fully developed, both thermally and mechanically;
2. the pressure drop (and from it the friction factor) was measured;
3. Seale's apparatus geometry (a span of rods between plates) has been studied by a number of other authors, thus corroborating data is available;
4. a range of Reynolds numbers and pitch-to-diameter ratios were investigated;
5. although spacer grids were present, the experiment was designed to minimize, rather than study, their impact on mixing; and
6. the domain is relatively simple to model.

Other datasets, in particular some by Rehme [7, 16, 19], Möller [48], Krauss [4] and Meyer [5], also ranked highly. Rather than simulate these datasets directly, the

Table 5.1: Geometry Data for Seale's Apparatus

parameter	Duct			units
	3	4	5	
number of rods	3	4	5	
rod diameter, D	50	50	50	[mm]
p/d ratio, γ_p	1.833	1.375	1.1	
duct width	275	275	275	[mm]
duct height	137.5	90.2	68.6	[mm]
gap width, b	41.6	18.7	5.0	[mm]
hydraulic diameter, D_h	125.0	57.6	27.1	[mm]

information provided by these references were used to corroborate the Seale data. Many of these datasets were discussed in the literature review (Chapter 2).

5.2 Final Validation Study Dataset

5.2.1 Description of Experiment

Seale [37] studied fully developed turbulent interchange mixing between rods by performing an experiment consisting of a single row of smooth, unheated rods placed between two horizontal plates (Figure 5.1). By producing a known heat flux in the top plate and holding the bottom plate at a constant temperature, Seale was able to determine the amount of thermal mixing between the rods after measuring the bulk coolant temperature above and below the rods.

Seale investigated three different duct geometries, each with a different pitch-to-diameter ratio, γ_p . In all three cases, 50 mm diameter rods were arranged in a horizontal row within a rectangular duct. Half-rods located at the lateral sides of the duct were used to simulate an infinite stretch of rods. Table 5.1 summarizes the geometric data for each of the three ducts, while Figure 5.2 provides schematic cross-sections of all three ducts. The duct numbering scheme begins at '3' to be consistent with Seale.

The working fluid was air. The inlet flow was allowed to reach mechanically fully developed conditions over the 200 hydraulic diameter length of the test section. For each duct, a range of Reynolds numbers from 3×10^4 to 3×10^5 were obtained by varying the inlet air mass flow rate.

The simulated fuel rods were constructed of an unidentified insulating material. Other investigators (*e.g.* Hetsroni *et al.* [26]) used acrylic plastic rods to investigate heated air

Figure 5.1: Detail of 5 Rod Duct ($\gamma_p = 1.1$)

Figure 5.2: Three Ducts used by Seale

Table 5.2: Measurement Uncertainties Reported by Seale

top wall heat flux	$\pm 1\%$
rod position	$< 1 \text{ mm}$
pressure	$\pm 6.7 \text{ Pa}$
temperature	$\pm 0.5 \text{ K}$
pressure/temperature probe position	$< 0.1 \text{ mm}$
gap Stanton number	$\pm 11\%$

flow and found heat conduction through the rods to be an insignificant source of error. Seale [37] reports a rod conduction heat ‘leakage’ of 2%.

Seale preheated the inlet air flow using a “special preheater” which imposed an inlet temperature profile close to the observed exit temperature profile. This allowed thermal development of the air to take place within the 200 hydraulic diameter length of the test section.

Electrical Joule heating of the top plate was adjusted by varying the current flow to the plate. When Seale observed no axial increase in bulk fluid temperature, it was asserted the heat flux from the top plate exactly balanced the heat transport through the gap and eventual heat removal through the constant-temperature bottom plate. Thus the measured top plate Joule heat was used as the measured gap mixing heat flux, q'' . Combined with measurements of the bulk temperature in the upper and lower subchannels, the gap Stanton number, St_g , was calculated.

Seale reported bulk fluid temperature (above and below the gap between the rods), Fanning friction factor, ratio of maximum axial velocity to rod/rod and rod/wall gap velocity, and gap Stanton number. For one geometry and Reynolds number ($\gamma_p = 1.375$, $Re = 9.07 \times 10^4$), Seale also published axial velocity and temperature contours. Table 5.2 summarises the measurement uncertainties reported by Seale [37].

5.2.2 Solution Domain and Boundary Conditions

Taking advantage of the horizontal periodicity of the test section, the solution domain consisted of a small vertical slice that incorporates half a rod and half a gap (Figure 5.1).

A structured mesh was used to discretize the domain. Based upon experiences from the preliminary validation, a number of requirements were specified for the mesh. First, the flow nodes closest to the walls (top, bottom, and rod surface) were placed in the

Figure 5.3: Cross sections of meshes used for final validation

(Note that the scale for each mesh is different; the rod diameter is 50 mm for all three meshes)

dimensionless range $30 < y^+ < 100$. Since y^+ is a function of Reynolds number, a different mesh was required for each inlet mass flow rate. Second, the control volume density in the gap region was increased to capture the velocity and temperature gradients expected in the gap region. Third, the aspect ratio of all elements was kept below 50:1, while the skew of all elements was kept in the range of 30 to 150 degrees.

Figure 5.3 provides typical mesh cross-sections for the three, four, and five-rod ducts. Table 5.3 geometry provides geometry details for the three meshes. Appendix G provides details about the mesh construction.

The properties of air at 300 K were used, as summarized in Table 5.4. Although air density decreases by approximately 15% from 300 K to 375 K (the maximum temperature measured by Seale), and molecular viscosity increases by a similar amount, properties were assumed constant for this investigation. This is justified for three reasons. First, use of constant properties facilitates a cost-saving separation of the flow and thermal solutions, as discussed in the next subsection. Second, diversion cross flow mixing (as caused by density variations) is not being studied. Third, turbulent viscosity is expected to

Table 5.3: Mesh Geometric Properties

Property	Duct #		
	3	4	5
γ_p	1.833	1.375	1.1
Axial (ID) nodes	150		
Radial (JD) nodes	15		
Azimuthal (KD) nodes	55		
Total control volumes	112,644		
Control volumes in cross-section	756		
Domain Length / D_h	8	17	37
Maximum aspect ratio in cross-section	7.68	6.40	9.63
in axial direction	8.38	14.2	51.2
Minimum skew (degrees)	31.6	36.3	38.9
Maximum skew (degrees)	148	142	138

Table 5.4: Fluid Properties for Final Validation Dataset [47]

Property	Value	Units
fluid	air	
density, ρ	1.1614	$[kg/m^3]$
molecular viscosity, μ	1.846×10^{-5}	$[Pa \cdot s]$
molecular thermal conductivity, Γ	2.63×10^{-2}	$[W/m \cdot K]$
specific heat capacity, c_p	1007	$[J/kg \cdot K]$

dominate over molecular values, therefore changes in molecular viscosity will be negligible. A similar argument is made pertaining to the molecular thermal conductivity, which increases by 22% between 300 K and 375 K. The heat capacity increases less than 1%, however.

Stationary wall boundary conditions were applied to the upper and lower walls, as well as the rod surface. The treatment of the wall boundary conditions for the turbulence equations was the same as for the preliminary validation (*i.e.* law of the wall). The top wall used a specified heat flux boundary condition, while the bottom wall was set to a constant temperature of 300K.

The inlet boundary condition consisted of a specified mass flux and a uniform velocity profile. Table 5.5 summarizes the inlet mass flow values investigated. These mass flows match the values used by Seale.

Table 5.5: Summary of Final Validation Inlet Mass Flows

geometry	mass flow [kg/s]	Reynolds number
$\gamma_p = 1.1$	0.021	3.44×10^4
	0.030	4.87×10^4
	0.051	8.25×10^4
	0.080	1.30×10^5
	0.100	1.62×10^5
	0.127	2.06×10^5
	0.184	3.00×10^5
$\gamma_p = 1.375$	0.031	4.59×10^4
	0.038	5.61×10^4
	0.050	7.25×10^4
	0.062	9.10×10^4
	0.077	1.14×10^5
	0.109	1.60×10^5
	0.203	3.00×10^5
$\gamma_p = 1.833$	0.027	3.44×10^4
	0.036	4.63×10^4
	0.056	7.15×10^4
	0.078	9.99×10^4
	0.128	1.62×10^5
	0.162	2.06×10^5
	0.235	3.00×10^5

The inlet turbulence intensity was specified as 5%, while the inlet turbulent length scale was specified as equal to the gap width.

The outlet condition was specified as a constant relative pressure of zero at a single control volume face at the outlet. Care was taken *not* to specify a uniform pressure of zero at the outlet as this would force fully-developed conditions at the outlet, whereas this may not be the case.

Symmetry boundary conditions were applied along the lateral sides of the domain.

5.2.3 Solution Methodology

Following the construction of the mesh, a methodology was followed to accurately simulate the conditions of Seale's experiment. The solution methodology was divided into two stages. In the first stage, the velocity, pressure, and turbulence fields under isothermal conditions were calculated. Due to the unique circumstances provided by Seale's experiment, the temperature solution could be 'split' from the mechanical flow solution and solved in a more efficient, two-dimensional domain. Once the turbulence field was obtained, the second stage consisted of calculating the temperature profile.

Details about this solution methodology are discussed in the next two subsections.

Mechanical Flow Solution

Although the flow is not fully developed after several hydraulic diameters, this length was sufficient to estimate for a given mesh the non-dimensional distance of the near-wall flow nodes. If the nodes were observed as too close to or too far from the wall (*i.e.* $y^+ < 30$ or $y^+ > 100$), the mesh was altered accordingly and the flow solution recalculated.

If the near-wall nodes were found to be in an acceptable range, the nodal velocity and turbulence fields (U, V, W, k , and ϵ) at the outlet were saved to a file. This file was used as the inlet condition for a second solution of the domain. This effectively doubled the length of the solution domain without actually solving the larger domain all at once. This provided a significant memory and time savings because it allowed the adequacy of the positioning of the flow nodes closest to the wall to be checked without performing a long run. This outlet rewinding technique was used also in the preliminary validation studies involving flow in circular pipes (Chapter 4).

Care was taken using this technique. The outlet solution was not rewound until the mass residual was sufficiently small ($\approx 10^{-6}$). This is because any mass residual is manifested as an error in the velocity field, an error which would be re-introduced to the system when the outlet field was rewound.

The convergence criteria for all code executions was a maximum residual of 5×10^{-5} or less for each of the U , V , W , and energy fields. This is a stricter solution convergence than the maximum residual of 1×10^{-4} or less used in the preliminary validation studies.

Thermal Solution

A challenging aspect of simulating Seale's experiment was Seale's use of a 'special pre-heater' which imposed a temperature profile on the inlet flow. According to Seale this profile closely matched the fully developed temperature field. Seale substantiates this by observing that the outlet temperature bulk was the same as the inlet, despite the fact heat was added from the top electrical plate. This would imply the heat added from the top plate was balanced by both thermal mixing in the gap and heat removal through the constant temperature bottom wall. Seale uses this property of his experiment (the heat flux from the top wall is balanced by the mixing in the gap) to measure the mixing in the gap. This unique balance of axial and cross-flow heat transfer can be used in an advantageous manner.

Under the boundary conditions imposed by Seale's experiment coupled with the $k - \varepsilon$ model's inability to predict secondary flow of the second kind, the thermal solution which would be eventually obtained by the code (if the domain was long enough to fully develop the thermal field) is two dimensional and non-convective. This can be demonstrated by considering the time-averaged energy equation solved by the code. Mixing Cartesian notation with vector for convenience, the energy equation can be written as:

$$\rho c_p \left(\frac{\partial T}{\partial t} + U \frac{\partial T}{\partial x} + V \frac{\partial T}{\partial y} + W \frac{\partial T}{\partial z} \right) = \nabla \Gamma_{eff} \cdot \nabla T + \dot{q}''' \quad (5.1)$$

Seale's experiment provides the following conditions (steady, fully developed, non-reactive flow):

$$\frac{\partial}{\partial t} = 0 \quad \text{and} \quad \frac{\partial}{\partial x} = 0 \quad \text{and} \quad \dot{q}''' = 0 \quad (5.2)$$

The absence of predicted secondary flow imposes the following additional conditions:

$$V = W = 0 \quad (5.3)$$

Therefore, the energy equation as modeled for the Seale experiment reduces to:

$$\begin{aligned} \nabla \Gamma_{eff} \cdot \nabla T &= \frac{\partial}{\partial y} \Gamma_{eff} \frac{\partial T}{\partial y} + \frac{\partial}{\partial z} \Gamma_{eff} \frac{\partial T}{\partial z} \\ &= 0 \end{aligned} \quad (5.4)$$

This is simply the equation for steady, two-dimensional heat conduction with isotropic, spatially-varying conductivity. Given the code calculated Γ_{eff} field, solving Equation (5.4)

provides the fully-developed temperature profile. The absence of velocity variables in Equation (5.4) allows the two-dimensional temperature field to be solved after, rather than concurrent with, the flow solution.

In the presence of either secondary flow or a non-zero axial change in temperature (therefore $V = W = \partial/\partial t \neq 0$) the flow and temperature calculations cannot be separated.

Appendix H provides details about the code modifications required to support this temperature solution.

The convergence criterion for the temperature solution was similar to that used for the mechanical solution: a maximum residual of 5×10^{-5} or less at all nodes in the domain.

5.3 Validation Study Results

5.3.1 Axial Velocity Distribution

Figures 5.4 through 5.6 provide contours of the axial velocity, U . For each pitch-to-diameter ratio, a small Reynolds number and large Reynolds number case is shown. The ratio of the maximum velocity, U_{max} to the bulk velocity, U_b is also shown.

Figures 5.4 through 5.6 indicate that the position of maximum axial velocity moves towards the gap as the pitch-to-diameter ratio increases. Also, the ratio of the maximum velocity to bulk velocity decreases with both γ_p and the Reynolds number. The decrease in U_{max}/U_b with Reynolds number is indicative of an increase in turbulent eddy diffusivity because velocity gradients are inversely proportional to this quantity.

Figure 5.7 compares measured and code predicted axial velocity contours ($\gamma_p = 1.375$, $Re=9.067 \times 10^4$). Both contours are normalized to the maximum velocity. While the contours near the top and bottom walls compare favourably, the code predicted velocity in the gap is lower. This ‘pushes’ the code predicted maximum velocity contours further from the gap than observed in the measured contours.

Table 5.6 summarizes the ratio of the axial velocity in the centre of the rod/rod gap, U_g , and rod/wall gap, U_w , to the maximum axial velocity for a Reynolds number of approximately 90,000. Table 5.6 indicates the code underpredicts the axial velocity in both the rod/rod and rod/wall gaps, with the largest underprediction observed for the tightest-packed rod duct ($\gamma_p = 1.1$). As the rods are moved further apart, the gap velocities approach the maximum velocities, and the code prediction error decreases. Note the observation from Figure 5.7 that the code underpredicts the axial velocity in

Figure 5.4: Axial Velocity Contours, $\gamma_p = 1.1$ Figure 5.5: Axial Velocity Contours, $\gamma_p = 1.375$

Figure 5.6: Axial Velocity Contours, $\gamma_p = 1.833$ Figure 5.7: Normalized Axial Velocity Contours, $\gamma_p = 1.375$, $Re=9.067 \times 10^4$ (normalized to maximum velocity)

Table 5.6: Measured and Predicted Ratios Gap Velocity Ratios, $Re \approx 90,000$

	Measured		Predicted		Difference	
	U_g/U_{max}	U_w/U_{max}	U_g/U_{max}	U_w/U_{max}	U_g/U_{max}	U_w/U_{max}
$\gamma_p = 1.1$	0.849	0.876	0.475	0.706	-44%	-19%
$\gamma_p = 1.375$	0.904	0.875	0.853	0.852	-5.6%	-2.6%
$\gamma_p = 1.833$	0.950	0.921	0.935	0.894	-1.6%	-2.9%

the gap is confirmed. Also note that although Seale's contour in Figure 5.7 suggests U_g/U_{max} is slightly less than 0.90, Seale's tabular data reports a value slightly greater than 0.90. This small discrepancy is attributed to Seale's undisclosed contour plotting technique, and the tabular data is considered more accurate.

The azimuthal gradient of axial velocity near the gap (*i.e.* the change in axial velocity from a point outside the gap to a point in the gap) is roughly approximated by U_g/U_{max} . The smaller the value of the ratio U_g/U_{max} , the larger the azimuthal gradient of axial velocity.

Velocity gradients are governed by the local turbulent diffusivity. Large turbulent diffusivities increase momentum diffusion, which in turn flattens gradients. Turbulent kinetic energy, however, is produced by velocity gradients. In other words, a turbulence field (and therefore a turbulent diffusivity field) represents the balance between the opposing effects of turbulence production and momentum diffusion. An accurate turbulence model will find the same balance as observed in experiment.

In this investigation, the underprediction of axial velocity in the gaps is indicative of an overprediction of the axial velocity's azimuthal gradient in the neighbourhood of the gap. This implies the turbulent eddy diffusivity in the gap is underpredicted. The next subsection describes the turbulent eddy diffusivity field by exploring the distribution of effective turbulent thermal conductivity, Γ_{eff} .

5.3.2 Effective Turbulent Thermal Conductivity, Γ_{eff}

The effective thermal conductivity, Γ_{eff} is the sum of a molecular conductivity component, Γ , and a turbulent component:

$$\Gamma_{eff} = \Gamma + \frac{c_p}{Pr_t} \frac{\rho c_\mu k^2}{\varepsilon} \quad (5.5)$$

where Γ is the molecular conductivity, and Pr_t is the turbulent Prandtl number, a constant equal to 0.9 in this investigation [59].

Turbulent eddy viscosity (or diffusivity), μ_t , equals $\rho c_\mu k^2/\varepsilon$. Thus,

$$\Gamma_{eff} = \Gamma + \frac{c_p \mu_t}{Pr_t} \quad (5.6)$$

Because Γ and Pr_t are constant, the distribution of effective thermal conductivity differs from the distribution of turbulent eddy diffusivity by a scaling factor and an additive constant. Thus observations pertaining to the distribution of Γ_{eff} can be used to make conclusions about the distribution of μ_t .

Figures 5.8 through 5.10 provide contours of the turbulent component of effective thermal conductivity normalized to the molecular conductivity:

$$\Gamma_t^{norm} = \frac{\frac{1}{Pr_t} \frac{\rho c_\mu k^2}{\varepsilon}}{\Gamma} \quad (5.7)$$

Figures 5.8 through 5.10 show a small Reynolds number and large Reynolds number contour of Γ_t^{norm} for each pitch-to-diameter ratio. Note that the contour scale is different for each pitch-to-diameter ratio.

In the case of $\gamma_p = 1.1$, the location of maximum effective thermal conductivity is not in the gap, but immediately above and below the gap. This is consistent with the turbulent axial velocity fluctuations observations made by Rehme [16] (Figure 2.2 in Section 2). Rehme also observed maximum turbulent transverse velocity fluctuations (*i.e.* v') in the gap centres. Therefore the turbulent thermal conductivity predicted by the code, as demonstrated by Figures 5.8 through 5.10, follow Rehme's observations for axial, rather than transverse, velocity fluctuation behaviour.

Near the walls, the turbulence intensity is lower and the turbulent thermal conductivity approaches the molecular value (*i.e.* the normalized value approaches 1). The turbulence decreases towards the walls, as expected by near-wall behaviour.

Rehme observed a low intensity area near the core of the subchannel, at the location of maximum axial velocity. Although Figures 5.8 through 5.10 do not exhibit a low-intensity region in the same area, a region of lower effective thermal conductivity is observed nearby, along the symmetry line.

As the pitch-to-diameter ratio increases, the location of maximum turbulent thermal conductivity moves further from the gap and towards the subchannel core. In addition, increasing the pitch-to-diameter ratio decreases the maximum turbulent thermal conductivity (all three pitch-to-diameter ratio cases are normalized to the same value of the molecular conductivity, Γ).

Increasing the Reynolds number also increases the turbulent thermal conductivity. For the $\gamma_p = 1.1$ case, the maximum normalized turbulent thermal conductivity is 90

Figure 5.8: Normalized Turbulent Thermal Conductivity Contours, $\gamma_p = 1.1$

Figure 5.9: Normalized Turbulent Thermal Conductivity Contours, $\gamma_p = 1.375$

times the molecular for $Re=48,700$, and increases to 460 times for $Re=299,600$. For $\gamma_p = 1.833$, the maximum normalized turbulent thermal conductivity is 40 times the molecular for $Re=46,300$ which increases to 200 times for $Re=299,600$.

The turbulent thermal conductivity in the gap core was observed to range from 40 to 100 times the molecular conductivity for $\gamma_p = 1.1$, with a maximum of over 450 times slightly outside the gap. The larger pitch-to-diameter cases exhibited lower maximum turbulent thermal conductivities, but the values in the gaps were higher than that of $\gamma_p = 1.1$. In other words, the lower pitch-to-diameter ratio cases exhibit a stronger variation in effective thermal conductivity vertically through gap than do the larger pitch-to-diameter ratio cases.

The next subsection presents the temperature fields which result from solving these effective thermal conductivity fields.

5.3.3 Temperature Fields

The previous section provided normalized contours of the turbulent component of effective thermal conductivity. These isotropic conductivity fields produce the temperature fields shown in Figures 5.11 through 5.13. For each pitch-to-diameter ratio, a small Reynolds number and high Reynolds number contour are shown. Each profile is normalized using the maximum and minimum fluid temperatures. Invariably, maximum temperatures were located at the top wall, while minimum temperatures were equal to the constant temperature bottom wall (300K). The minimum-to-maximum ΔT for each contour (with a wall heat flux of $1000 [W/m^2 \cdot K]$) is provided.

The change in temperature gradients across the gap as a function of the pitch-to-diameter can be seen in Figures 5.11 through 5.13. While the normalized temperature contours are virtually independent of the Reynolds number, the maximum temperatures for the higher Reynolds number cases are lower than that of lower Reynolds number cases. In other words, although the normalized gradients are the same, the dimensional temperature gradients across the gap are lower for larger Reynolds numbers. The independence of temperature on Reynolds number arises from the disappearance of a convection term in each of the energy, k , and ϵ equations. The production term P_k in the energy equation does not produce a Reynolds number following non-dimensionalization.

As the pitch-to-diameter ratio is increased, a more gradual change in top-to-bottom temperature profile is observed. This is the result of a combination of two factors. The first factor is related to the effective thermal conductivity field. As illustrated in Figures 5.8 through 5.10, larger values of γ_p exhibit higher values of effective thermal

Figure 5.10: Normalized Turbulent Thermal Conductivity Contours, $\gamma_p = 1.833$ Figure 5.11: Normalized Temperature Contours, $\gamma_p = 1.1$, $q'' = 1000$ W

Figure 5.12: Normalized Temperature Contours, $\gamma_p = 1.375$, $q'' = 1000$ W Figure 5.13: Normalized Temperature Contours, $\gamma_p = 1.833$, $q'' = 1000$ W

Figure 5.14: Normalized Temperature Contours, $\gamma_p = 1.375$ (normalized to maximum temperature)

conductivity in the gap. Because the temperature gradient is proportional to the conductivity the larger values of γ_p exhibit a more gradual change in the temperature profile vertically across the gap. The $\gamma_p = 1.1$ case, however, exhibits higher effective conductivity above and below the gap. The smaller pitch-to-diameter case exhibits a flatter temperature gradient in these regions above and below the gap.

The second factor for the flatter temperature gradient for larger values of γ_p is related to the geometry itself. Because the duct temperature is fully developed and steady, the total vertical heat flow at each horizontal elevation is constant and equal to the heat flow from the top wall. In the gap, the flow area is constricted, therefore the heat flux, q'' increases. The temperature gradient in the gap steepens as per Fourier's heat conduction law. Smaller gaps, therefore, are expected to demonstrate larger temperature gradients across the gap (for the same diffusivity). As observed in the previous section however, effective thermal conductivity is in general higher for small-gap geometries, which works towards flattening the gradient. The temperature gradient across the gap is the result of a balance between the opposing influences of gap heat flux (which decreases with gap size) and effective thermal conductivity (which also decreases with gap size).

Figure 5.14 compares the code predicted temperature contours for $\gamma_p \approx 1.375$ with those measured by Seale. Both the Seale and code predicted results are normalized to the minimum and maximum temperatures.

Comparison of the measured and code predicted temperature contours in Figure 5.14 reveals the code predicted temperature gradient across the gap is overpredicted. In the distance over which the code predicted a decrease in normalized temperature from 0.80 to 0.20, the measured normalized temperature decreased from 0.65 to 0.40. This represents an approximately 140% overprediction in temperature gradient across the gap. Because gap mixing flattens gradients, the observed overprediction in temperature gradient suggests an underprediction of turbulent interchange mixing.

Both the measured and code predicted normalized temperature contours exhibit a normalized temperature of 0.5 in the gap, indicative of top-to-bottom symmetry. Further, the measured temperature contours intercept the rod surface at roughly right-angles, indicative of adiabatic conditions. The lateral symmetry surfaces in the measured contour plot also exhibit adiabatic conditions, thus supporting the use of horizontal periodicity symmetry for the code predictions.

5.3.4 Wall Shear

The variation in wall shear around the pin surface was graphed by using the near-wall values of the turbulent kinetic energy, k , to calculate τ_w :

$$\tau_w = \rho \sqrt{c_\mu} k \quad (5.8)$$

where $c_\mu = 0.09$. Therefore the variation in wall shear near the gap is proportional to the variation in turbulent kinetic energy, k .

Figures 5.15 through 5.17 illustrate the code predicted variation in wall shear around the rod normalized to the average rod wall shear. The angle $\theta = 0$ degrees corresponds to the surface of the rod facing into the rod/rod gap, while $\theta = 90^\circ$ degrees corresponds to the surface of the rod facing into the rod/wall gap (refer to Figure 2.4 in Section 2.2.5).

Included in Figure 5.15 is the data reported by Rehme [7] for wall subchannels with a pitch-to-diameter ratio of 1.07 and a Reynolds number of 8.7×10^4 . Data reported by Krauss and Meyer [4] for $\gamma_p = 1.12$ and $Re = 65,00$ are also included in the figure.

Comparing the experimental data with the code predictions for $\gamma_p = 1.1$ suggest the code underpredicts the wall shear in the gap (where $\theta = 0$ degrees). As per Equation (5.8), this is indicative of an underprediction of turbulent kinetic energy in the gap. In compensation, the code overpredicts the shear near the wall facing into the flow (*i.e.* angles between 30 and 60 degrees). The underprediction of the shear in the gap region is cause for concern because an underprediction of the turbulent kinetic energy in the gap is expected to result in underprediction of turbulent interchange mixing. This is because turbulent interchange mixing is governed by turbulent fluctuations in the gap.

Figure 5.15: Normalized Wall Shear Around Rod, $\gamma_p = 1.1$

The average wall shear measured by Rehme and Krauss and Meyer were not provided. Calculation of the friction factor in the next Chapter, however, will indicate that the predicted average wall shear compares to Seale's data within measurement uncertainty.

The angle at which the predicted maximum wall shear occurs is approximately 41 degrees from the gap and is constant with respect to Reynolds number. This position of maximum wall shear is consistent with the experimental data of both Rehme [7] and Krauss and Meyer [4].

The cusp observed in the code predicted wall shear at 51 degrees is an artifact of the mesh topology. At this location, a control node is used to fix the distance of the near-wall nodes from the rod wall. The elliptical interpolation of the nearby nodes results in a small cusp in the locus of near-wall nodes at this location. Mesh refinement in this location may eliminate this cusp. Because this location is relatively far from the gap, however, the observed discontinuity is not expected to influence predictions of turbulent interchange mixing.

Figure 5.16, where $\gamma_p = 1.375$, exhibits a behaviour different from that of $\gamma_p = 1.1$. While the distribution is flatter (as is expected from wider-spaced rods [18]), there is a definite movement of the location of peak wall shear towards the gap ($\theta = 0$) as the

Figure 5.16: Normalized Wall Shear Around Rod, $\gamma_p = 1.375$

Reynolds number increases. This is consistent with Carajilesov and Todreas' observation that the position of maximum wall shear moved into the gap as γ_p increased [18]. This suggests that the location of maximum turbulent kinetic energy moves from outside the gap (as observed in Figure 5.15) into the gap core. Figure 5.17 suggests that for $\gamma_p = 1.833$, the maximum wall shear is observed in the gap for the entire range of Reynolds numbers investigated. Because wall shear is proportional to the radial gradient of axial velocity, this observed movement of the position of maximum wall shear into the gap for larger values of γ_p is consistent with the observed movement of the maximum velocity towards the gap for larger values of γ_p .

5.4 Summary

The results of the simulation of Seale's experiment produced the following results.

The axial velocity profiles indicate an underprediction of the axial velocity in the rod/rod and rod/wall gaps, with the largest underprediction observed for the most tightly packed rod case ($\gamma_p = 1.1$).

Contours of normalized turbulent component of thermal conductivity revealed the

Figure 5.17: Normalized Wall Shear Around Rod, $\gamma_p = 1.833$

position of maximum thermal conductivity moved from just outside the gap for $\gamma_p = 1.1$ to nearer the subchannel core for $\gamma_p = 1.833$. The conductivity in the middle of the gap, however, was observed to be lower for $\gamma_p = 1.1$ than for larger pitch-to-diameter ratios.

A novel approach to solving the temperature field was employed. This approach used the two dimensional, steady nature of the thermal boundary conditions to solve the temperature field after, rather than coupled with, the velocity and turbulence fields. The normalized temperature fields for each rod pitch-to-diameter ratio were largely independent of Reynolds numbers. The magnitude of the top-to-bottom temperature difference, however, decreased with Reynolds number and gap mixing improved.

The circumferential variation in wall shear exhibited a larger minimum-to-maximum variation for $\gamma_p = 1.1$ than that measured by Rehme [7] and Krauss and Meyer [4]. The position of maximum wall shear, however, was predicted well. For $\gamma_p = 1.375$, the position of maximum wall shear moved into the core of the gap as the Reynolds number increased. In the case of $\gamma_p = 1.833$, the maximum wall shear position was observed in the gap for all Reynolds number values investigated.

The next chapter analyses the velocity and temperature fields by comparing code predicted friction factors and turbulent interchange mixing with the experimental results.

Chapter 6

Analysis of Validation Results

6.1 Overview

The previous chapter provided validation of code predicted velocity, temperature, and wall shear results. This chapter uses these results to calculate the integrated quantities of friction factor and turbulent interchange mixing. Analysis of these results is provided, with specific effort made to determine the underlying source of the computational model's strengths and weaknesses.

6.2 Predicted Friction Factor

The friction factor for each case was calculated from the predicted constant pressure gradient. Figures 6.1 through 6.3 compare the code predicted friction factors with those measured by Seale [37]. Friction data for Duct 5 was not provided by Seale due to an error during the measurement of pressure.

Also included in Figures 6.1 through 6.3 is Cheng and Todreas's friction factor correlation for wall subchannel geometries [8]. The wall subchannel correlation was chosen due to the presence of flat walls in Seale's apparatus. In general, both the code predicted and experimentally observed friction factors have a strong Reynolds number dependence than Cheng and Todreas' correlation. Nevertheless, the magnitude of the measured and predicted friction factors are close to Cheng and Todreas's results, particularly for larger values of γ_p .

Figures 6.1 through 6.3 include curve fits for the code predicted and experimentally measured friction factors. These curve fits were obtained by performing a linear regression of the logarithm of friction versus the logarithm of Reynolds number. This provided an

Figure 6.1: Predicted Friction Factors for Seale Experiment Duct 5, $\gamma_p = 1.1$ Figure 6.2: Predicted Friction Factors for Seale Experiment Duct 4, $\gamma_p = 1.375$

Figure 6.3: Predicted Friction Factors for Seale Experiment Duct 3, $\gamma_p = 1.833$

expression of the form $f = a_f \text{Re}^{b_f}$, which is used by many authors to derive one mixing model form or another. Table 6.1 summarizes the values of the curve fits along with standard errors for each constant. The standard error in the predicted values, S_{err} , is estimating using the following [60]:

$$S_{err} = \sqrt{\left[\frac{1}{n(n-2)} \right] \left\{ n \sum y^2 - (\sum y)^2 - \frac{[n \sum xy - (\sum x)(\sum y)]^2}{n \sum x^2 - (\sum x)^2} \right\}} \quad (6.1)$$

where n is the number of points, x is the observed values and y is the predicted values.

In general, the the code predicted curve fit standard error is lower than that of the experimentally observed curve fit. This is likely due to the higher precision of the code (*i.e.*, the ability for the code to recreate results without scatter)¹.

The code predicted values of a_f and b_f overlap the experimentally observed values within the standard error. In particular, for $\gamma_p = 1.833$ the code predicted and experimental values of a_f and b_f are nearly identical. In Figure 6.3, the two curves are virtually indistinguishable.

The good agreement between the code predictions of the friction factor and measured

¹Precision implies lack-of-scatter around a mean, while accuracy implies proximity of the mean to the 'true' value.

Table 6.1: Results of Linear Regression of Friction Factor Results

	$f = a_f Re^{b_f}$			
	Experiment [37]		Code Prediction	
	a_f	b_f	a_f	b_f
Duct 5 ($\gamma_p = 1.1$)	n/a	n/a	0.0689 ± 0.0175	-0.237 ± 0.020
Duct 4 ($\gamma_p = 1.375$)	0.0912 ± 0.0479	-0.261 ± 0.037	0.09853 ± 0.045	-0.264 ± 0.032
Duct 3 ($\gamma_p = 1.833$)	0.0718 ± 0.0598	-0.237 ± 0.052	0.0680 ± 0.010	-0.232 ± 0.012

values is indicative of good predictions of near-wall behaviour. Given that the literature review concluded that the law of the wall is applicable to rod bundle geometries and such a law is used as the boundary condition for the momentum equation, the good agreement of the friction factor results is not surprising. While the circumferential distribution of wall shear is for $\gamma_p = 1.1$ did not match experimental measurements very closely (Chapter 6), the friction factor agreement indicates that the average wall shear is predicted correctly.

6.3 Turbulent Interchange Mixing

Using the code predicted temperature and velocity fields in conjunction with the top-wall heat flux, the gap Stanton number, St_g , for each case was obtained.

$$St_g = \frac{q'}{b(T_b^{top} - T_b^{bottom}) \rho c_p U_b} \quad (6.2)$$

Bulk temperatures were calculated for the top and bottom halves of the domain using a formula similar to that used in the preliminary validation investigation of heated pipe flow (Equation (4.11) in Chapter 4).

$$T_b = \frac{1}{A_t U_b} \sum_i A_i U_i T_i \quad (6.3)$$

where i is each control volume in the cross-section, A_i is the area of each control volume, and A_t is the total cross-sectional area of the duct.

Table 6.2 summarizes the code predicted upper and lower bulk temperatures for various cases along with the resulting gap Stanton numbers.

Included in Table 6.2 are various cases illustrating the relative insensitivity of the gap Stanton number to the choice of wall heat flux. This insensitivity arises because gap

Table 6.2: Code Predicted Gap Stanton Numbers

Case	Reynolds	Bulk Temperature [K]		$q''[W]$	St_g
		Upper Subchannel	Lower Subchannel		
Duct 5 $\gamma_p = 1.1$	3.44×10^4	969	325	1000	7.26×10^{-4}
		1238	334	1414	7.31×10^{-4}
	4.87×10^4	545	310	500	7.02×10^{-4}
		786	319	1000	7.05×10^{-4}
		987	326	1414	7.04×10^{-4}
		1272	337	2000	7.06×10^{-4}
		597	313	1000	6.83×10^{-4}
	8.25×10^4	718	317	1414	6.87×10^{-4}
		363	303	500	6.43×10^{-4}
		426	306	1000	6.46×10^{-4}
		477	308	1414	6.52×10^{-4}
	2.06×10^5	345	302	500	6.27×10^{-4}
		389	304	1000	6.35×10^{-4}
		477	308	1414	6.40×10^{-4}
		345	302	500	6.27×10^{-4}
Duct 4 $\gamma_p = 1.375$	4.59×10^4	420	327	1000	2.67×10^{-3}
	9.10×10^4	423	319	1000	1.21×10^{-3}
	1.14×10^5	401	316	1000	1.18×10^{-3}
	1.60×10^5	375	312	1000	1.14×10^{-3}
	3.00×10^5	342	307	1000	1.10×10^{-3}
Duct 3 $\gamma_p = 1.833$	3.43×10^4	674	384	1000	1.49×10^{-3}
	4.63×10^4	600	368	1000	1.38×10^{-3}
	1.62×10^5	415	327	1000	1.04×10^{-3}
	2.06×10^5	395	323	1000	9.89×10^{-4}
	3.00×10^5	326	307	500	1.31×10^{-3}
		349	313	1000	1.38×10^{-3}
		398	326	2000	1.38×10^{-3}

Figure 6.4: Predicted Gap Stanton Numbers for Seale Experiment, $\gamma_p = 1.1$

mixing is a function of the fluid conductivity and turbulence fields and not a function of temperature. If the wall heat flux is changed, the difference between the upper and lower subchannel bulk temperatures is altered such that the gap Stanton number remains largely unchanged.

A general observation from Table 6.2 is that the difference between the upper and lower subchannel bulk fluid temperatures decreases with Reynolds number. This is a consequence of the larger effective thermal conductivity fields observed for larger Reynolds numbers.

Figures 6.4 through 6.6 compare the code predicted gap Stanton numbers with those obtained from Seale's experiment.

Clearly, the code underpredicts the gap Stanton number. In the case of $\gamma_p = 1.1$ (Figure 6.4), the underprediction exceeds an order of magnitude. As the pitch-to-diameter ratio increases (indicating wider rod spacing) the amount of underprediction is reduced. More specifically, the code predicted gap Stanton numbers increase slightly with γ_p , while Seale's measurements of St_g drop with γ_p .

Figures 6.4 through 6.6 include curve fits of both the code predicted and experimental gap Stanton numbers in the form $St_g = a_s Re^{b_s}$. Investigation of a relationship in this

Figure 6.5: Predicted Gap Stanton Numbers for Seale Experiment, $\gamma_p = 1.375$ Figure 6.6: Predicted Gap Stanton Numbers for Seale Experiment, $\gamma_p = 1.833$

Table 6.3: Results of Linear Regression of Gap Stanton Number Results

	$St_g = a_s Re^{b_s}$			
	Experiment [37]		Code Prediction	
	a_s	b_s	a_s	b_s
Duct 5 ($\gamma_p = 1.1$)	3.17×10^{-2} $\pm 4.2 \times 10^{-2}$	-0.106 ± 0.076	1.318×10^{-3} $\pm 1 \times 10^{-4}$	-0.057 ± 0.004
Duct 4 ($\gamma_p = 1.375$)	7.15×10^{-3} $\pm 1.1 \times 10^{-2}$	-0.0271 ± 0.083	4.02×10^{-3} $\pm 8 \times 10^{-4}$	-0.104 ± 0.015
Duct 3 ($\gamma_p = 1.833$)	5.53×10^{-3} $\pm 3.4 \times 10^{-3}$	-0.055 ± 0.042	1.56×10^{-2} $\pm 3 \times 10^{-4}$	-0.225 ± 0.002

form will assist the exploration of the dependence of mixing on the friction factor.

The code predicted curve fits are very precise as evidenced by the small standard error values. In the $\gamma_p = 1.833$ case, the gap Stanton number for a Reynolds number of 3×10^5 does not follow the $St_g = a_s Re^{b_s}$ trend and is therefore not included in the curve fit calculation. Note, however, this does not imply the gap Stanton number for $Re = 3 \times 10^5$ is in error. Rather, its non-compliance with a $f = a_s Re^{b_s}$ is noted and kept from altering the trend exhibited by the lower Reynolds number cases.

Error analysis of experimental data using the reported standard errors yields a variation of approximately 5% to 6% in the value of the gap Stanton number for $\gamma_p = 1.1$, 17% to 20% in St_g for $\gamma_p = 1.375$ and approximately 2% in St_g for $\gamma_p = 1.833$. The larger variation in gap Stanton number for $\gamma_p = 1.375$ arises from the larger standard error in b_s for this pitch-to-diameter ratio (*i.e.* the gap Stanton numbers do not follow the $St_g = a_s Re^{b_s}$ form as closely as the other two value of γ_p .)

Figure 6.7 compares the code predicted and measured gap Stanton number with subchannel models provided in the literature survey. The models reported as applicable to a wide range of subchannel geometries were used (Rogers and Rosehart [34], van Der Ros and Bogaardt [35], Rogers and Todreas [32]). The Seale and code prediction results were obtained using the $St_g = a_s Re^{b_s}$ curve fits with a Reynolds number of 10^5 . The error bars on the Seale results in Figure 6.7 were estimated from the scatter in the data reported by Seale.

The trend exhibited by the Seale's data is similar to that exhibited by both van Der Ros and Bogaardt [35] eddy viscosity model and Rogers and Todreas' gap Stanton model [32]. The code's underprediction of mixing is clear for $\gamma_p = 1.1$, however the $\gamma_p = 1.375$ and $\gamma_p = 1.833$ values agree with van Der Ros and Bogaardt's eddy viscosity

Figure 6.7: Comparison of code and experiment results with subchannel models

model to well within an order of magnitude. This is notable considering van Der Ros and Bogaardt investigated subchannel mixing with a geometry consisting of two square ducts connected laterally by a smaller rectangular duct. Their detailed measurements of the lateral temperature change in this orthogonal domain provided the data required to produce their model.

In summary, the code predicted turbulent interchange mixing is underpredicted by the code, particularly for smaller values of γ_p . The $\gamma_p = 1.375$ and $\gamma_p = 1.833$ results are closer to the experimental values, but match more reasonably with van Der Ros and Bogaardt's model.

6.4 Dependence of Mixing and Friction on Reynolds Number

The literature review discussed how many authors assert mixing is proportional to the square root of the friction factor. This is based on Nikuradse's relationship between

turbulent eddy diffusivity and friction.

$$\frac{\mu_t}{\rho} = \epsilon_{ij}^M \propto \text{Re} \sqrt{f} \quad (6.4)$$

As discussed in the literature review, most authors find or assume a $\text{Re}^{0.9}$ dependence of mixing. This arises from an expansion of Nikuradse's relationship assuming a dependence of $\text{Re}^{-0.2}$ of friction on Reynolds number.

The current investigation can potentially validate Nikuradse's relation (and all subsequent models based upon it) because a subchannel mixing model was not used. Both friction and mixing, although related *via* the turbulence field, were not explicitly linked, unlike most subchannel mixing models. By determining the dependence of mixing on Reynolds number, and separately the dependence of the friction factor on Reynolds number, the form of the relationship between mixing and friction can be determined.

Equation 2.26 in the literature review (Chapter 2) provides the relationship between eddy diffusivity and gap Stanton number.

$$\text{St}_g = \frac{D_h}{\text{Re} \delta_{ij}} \frac{\epsilon_{ij}^H}{\nu} \quad (6.5)$$

Thus, given Nikuradse's form, the relationship between gap Stanton number and friction is straightforward.

$$\text{St}_g \propto \sqrt{f} \quad (6.6)$$

Given a friction factor of the form $f = a_f \text{Re}^{b_f}$ and a Stanton number of the form $\text{St}_g = a_s \text{Re}^{b_s}$, the above equation implies that $b_f = 2b_s$.

The regression analysis of the measured and code-predicted friction factors and gap Stanton numbers are given in Tables 6.1 and 6.3 respectively. Table 6.4 compares the ratio of b_f to b_s for the curve fits obtained from Seale's experiment with that predicted by the code. Included in Table 6.4 are commonly used values of b_f and b_s , as discussed in the literature review (Chapter 2).

From Table 6.4 it is clear that neither Seale's experiment nor the code are able to confirm the square root relationship between the friction factor and gap Stanton number. The standard errors in Seale's measured gap Stanton numbers are large and therefore significantly reduce the quality of the comparison. The code-predicted standard errors are smaller, however only the $\gamma_p = 1.375$ case yields a code predicted ratio of b_f/b_s which includes the value of 2.0 within its error range.

Owing to the inaccuracy of the code predicted gap Stanton numbers coupled with the large scatter in Seale's measurements of St_g , this investigation can not confirm the relationship between mixing and friction factor assumed by many authors.

Table 6.4: Ratio of b_f to b_s

		Measured	Predicted	Common Value
$\gamma_p = 1.1$	b_f	n/a	-0.237 ± 0.020	-0.2
	b_s	-0.106 ± 0.076	-0.057 ± 0.004	-0.1
	b_f/b_s	n/a	4.16 ± 0.69	2.0
$\gamma_p = 1.375$	b_f	-0.261 ± 0.037	-0.264 ± 0.032	-0.2
	b_s	-0.0271 ± 0.083	-0.104 ± 0.015	-0.1
	b_f/b_s	9.63 ± 15.0	2.54 ± 0.79	2.0
$\gamma_p = 1.833$	b_f	-0.237 ± 0.052	-0.232 ± 0.012	-0.2
	b_s	-0.055 ± 0.042	-0.225 ± 0.002	-0.1
	b_f/b_s	4.31 ± 17.9	1.03 ± 0.06	2.0

6.5 Distribution of Turbulent Eddy Diffusivity in the Gap

In a previous section it was observed that the code predicted friction factor matched the measured values well. The gap Stanton number, however, was underpredicted. Both of these quantities are dependent on the turbulence field, in particular the turbulent eddy diffusivity. Exploration of the distribution of turbulent eddy diffusivity may uncover the reason why friction is predicted well but turbulent interchange mixing is modeled poorly.

The normalized turbulent eddy diffusivity, μ_t^+ , is calculated using the following:

$$\begin{aligned}
 \mu_t^+ &= \frac{\mu_t}{\rho \hat{r} U_\tau} \\
 &= \frac{c_\mu k^2}{\varepsilon \hat{r} U_\tau}
 \end{aligned} \tag{6.7}$$

where $\hat{r}$ is the distance between the rod wall surface and the locus of zero shear. Within the gap between the rods, $\hat{r}$ equals half the gap width because the location of zero shear is the midpoint between the two rods.

The code predicted variation of μ_t^+ across the gap (*i.e.* $\theta = 0$ in Figure 2.4 of Section 2) for each of the pitch-to-diameter ratios is provided in Figures 6.8 through 6.10. Included in the figures are Rehme's data for the radial component of μ_t for $\gamma_p = 1.1$ $Re=8.7 \times 10^4$ [7, 19] and Reichardt's model for circular tubes [12].

Figure 6.8 illustrates a good agreement between code predicted normalized eddy vis-

Figure 6.8: Predicted Normalized Eddy Viscosity, $\gamma_p = 1.1$ Figure 6.9: Predicted Normalized Eddy Viscosity, $\gamma_p = 1.375$

Figure 6.10: Predicted Normalized Eddy Viscosity, $\gamma_p = 1.833$

cosity for $\gamma_p = 1.1$ and Rehme's radial component data, particularly closer to the wall (*i.e.* $r/\hat{r} \rightarrow 0$). As γ_p increases (Figures 6.9 and 6.10), the normalized turbulent eddy viscosity approaches Reichardt's model for a circular pipe. This indicates the predicted turbulence field in the neighbourhood of a rod approaches circular pipe wall behaviour as the space between rods increases. The near-wall behaviour for both tightly and loosely packed rods, however, is similar and largely independent of Reynolds number.

The axial pressure drop arises from radial diffusion of momentum to the walls of the duct, and the near-wall turbulent eddy diffusivity governs this momentum transfer. In light of the good prediction of near-wall turbulent eddy diffusivity shown in Figures 6.8 through 6.10, it is not surprising the friction factor is predicted well.

One of the assumptions of the $k - \varepsilon$ model is the turbulence is in local equilibrium (production balances dissipation). The ability for the $k - \varepsilon$ model to accurately predict the radial component of μ_t suggests the near-wall turbulence is in equilibrium. The behaviour of the non-radial components, however, require further discussion.

6.6 Discussion of Isotropic Turbulent Eddy Diffusivity Model

Analysis of the numerically predicted final validation results indicates that the radial component of turbulent eddy diffusivity is predicted well by the code. As discussed in the literature review, however, the turbulent eddy diffusivity in rod bundle arrays is anisotropic.

Various investigators [28, 4, 16] found the azimuthal component of turbulent eddy diffusivity as large as 100 times the radial component, with the largest anisotropy factor occurring in the middle of the gap. While the isotropic eddy viscosity model used in the code predicts the radial component well, the azimuthal component is therefore underpredicted by as much as 100 times. It is the azimuthal component which governs mixing by turbulent interchange.

If an underprediction of the turbulent eddy diffusivity in the azimuthal direction is responsible for the underprediction of turbulent interchange mixing, a similar influence on the momentum solution should be observed.

The momentum analogue to underprediction of turbulent interchange mixing is underprediction of the axial velocity in the gap. The gradient $\partial U / \partial \varphi$ (*i.e.* the variation in axial velocity circumferential to the rod) is governed by turbulent eddy diffusivity in the azimuthal direction. Larger turbulent eddy viscosity values tend to reduce velocity

gradients. Therefore the observed underprediction in azimuthal turbulent eddy viscosity should lead to an overprediction in $\partial U/\partial \varphi$, particularly in the region of maximum turbulence anisotropy (*i.e.* the gap). Table 5.6 in Section 5.3.1 provided a comparison of the measured and predicted axial velocities in the gap, U_g , as a fraction of the maximum axial velocity, U_{max} . A lower value of the ratio U_g/U_{max} implies a larger gradient $\partial U/\partial \varphi$ in the gap. The underprediction in U_g/U_{max} observed in Table 5.6 confirms the expected overprediction in $\partial U/\partial \varphi$, and is therefore consistent with the premise of underprediction of azimuthal eddy viscosity.

As discussed in literature review (Section 2.6), Krauss and Meyer [4, 5] report a variation in the turbulent Prandtl number as high as 2.5, while this investigation assumes a constant value of 0.9. Increasing the turbulent Prandtl number, however, would reduce effective thermal conductivity therefore decreasing turbulent interchange mixing. Because the momentum solution is independent of Pr_t , however, the underprediction in gap velocity indicates that choice of turbulent Prandtl number alone is not responsible for the underprediction of turbulent interchange mixing.

Seale augmented an isotropic eddy viscosity model by multiplying the eddy diffusivity obtained from the $k - \varepsilon$ model by an anisotropy factor [11]. Specifically, Seale varied c_μ^φ (*i.e.* c_μ in the azimuthal direction) from a maximum of approximately $50c_\mu$ near the rod walls to a minimum of c_μ along the locus of maximum axial velocity. Seale assumed the c_μ^r (the radial component of c_μ) remained constant and equal to c_μ .

Seale found using such spatial variations improved code predictions somewhat, although the turbulent interchange mixing was still underpredicted. Yang and Chieng [61] used an identical method and virtually identical anisotropy distributions. Yang and Chieng found the anisotropy distribution which yielded the most satisfying results was similar to the distribution used by Seale. The distribution reported by both investigators was:

$$c_\mu^\varphi = c_\mu \left[A e^{-(3r/\hat{r})} + 1 \right] \quad (6.8)$$

where Seale used $A = 50$ while Yang and Chieng used $A = 30$.

Seale utilized nine different distributions of c_μ^φ/c_μ^r and found the diffusion of momentum to the walls and into the gap was largely insensitive to the choice of distribution. Working backwards, this implies that deduction of the exact variation of c_μ^φ/c_μ^r based on experimental measurement would be difficult.

A more rigorous approach to modeling the turbulence anisotropy would involve estimating the active components of the Reynolds stress tensor, $\overline{u_i' u_j'}$ separately. Launder and Spalding [59] suggest an algebraic stress model which is based upon the transport

equation for turbulent stress:

$$\frac{\partial \overline{u'_i u'_j}}{\partial t} + U_j \frac{\partial \overline{u'_i u'_j}}{\partial x_j} = - \left[\overline{u'_i u'_k} \frac{\partial U_j}{\partial x_k} + \overline{u'_j u'_k} \frac{\partial U_i}{\partial x_k} \right] + D_{ij} + \varepsilon_{ij} + R_{ij} \quad (6.9)$$

where D_{ij} , ε_{ij} and R_{ij} are the diffusive, dissipative, and redistributive components, respectively. The terms are approximated by assuming [59]:

- i) diffusional transport is proportional to the stress component gradient;
- ii) dissipation is isotropic in each of the three normal stresses and is zero for the shear stresses;
- iii) turbulent stress redistribution due to pressure fluctuations, R_{ij} , can be modeled using two terms: the first involving the product of Reynolds stress and k/ε ; the second involving products of stresses and mean velocity gradients.

By assuming the convective and diffusive components are zero, and observing the models of ε_{ij} and R_{ij} do not contain gradients of stress components, Equation (6.9) becomes an algebraic, rather than differential equation. This algebraic equation can be readily solved given appropriate boundary conditions.

It is not clear if use of an algebraic stress model of turbulence will improve the turbulent interchange mixing while maintaining the accuracy of the friction factor predictions. Clearly, improving turbulent interchange results at the expense of other quantities would not constitute progress. Further research into the implications of using such a turbulence model is strongly recommended.

6.7 Mesh Sensitivity Studies

Three studies were performed to determine the sensitivity of the results to mesh resolution, near-wall node placement and inlet turbulent parameters. The first study explored the variation of reported results as a function of mesh resolution (*i.e.* control volume size). The second study explored the influence of the position of the near-wall nodes on the reported results (*i.e.* sensitivity to y^+). The third study looked at independence of the mixing and friction results to selection in input turbulence parameters (*i.e.* inlet turbulence intensity and length scale).

Table 6.5: Mesh Resolution Sensitivity Parameters

	$\gamma_p = 1.1$		$\gamma_p = 1.375$		$\gamma_p = 1.833$	
	Base Case	Sens. Case	Base Case	Sens. Case	Base Case	Sens. Case
Axial (ID) nodes	150					
Radial (JD) nodes	15	9	15	9	15	9
Azimuthal (KD) nodes	55	43	55	43	55	43
Total control volumes	112,644	50,064	112,622	50,064	112,662	50,064
Control volumes in cross-section	756	344	756	344	756	344
Maximum aspect ratio in cross-section	9.63	8.18	6.40	9.58	7.68	6.53
Maximum aspect ratio in axial direction	51.2	30.2	14.2	11.1	8.38	6.53
Minimum skew (degrees)	38.9	38.9	36.3	36.3	31.6	31.6
Maximum skew (degrees)	138	138	142	142	148	147

6.7.1 Mesh Resolution and Near-Wall Node Position Sensitivity

A coarser mesh was constructed to explore the sensitivity of the predicted results to variations in mesh resolution. Table 6.5 summarises the base case and sensitivity mesh parameters. The coarser mesh used 54% less control volumes in each cross-section, but an equal number of axial control volumes. The near-wall nodes for the coarse mesh cases were located the same distance from the wall as for the large mesh cases (*i.e.* the same y^+ values were used).

The near-wall node sensitivity study investigated the impact of moving the near-wall nodes outside the recommended y^+ range of 30 to 100. For the sensitivity cases, the near-wall nodes in the gap regions were placed in the range $100 < y^+ < 200$. Sensitivity to placement of nodes in the region $y^+ < 30$ was not investigated because the computer program generates warnings when the nodes are moved too close to the wall.

Figures 6.11 through 6.13 compares the base case friction factors with those obtained from the mesh size and near-wall node sensitivity studies.

The variation in friction factor due to moving the near-wall nodes outside $y^+ > 100$ ranged from approximately -1.1% for $\gamma_p = 1.1$ to -4.8% for $\gamma_p = 1.833$. In general, the moving the near-wall nodes outside $y^+ > 100$ reduced the friction factor. Using the relation $\tau_w = \rho\sqrt{c_u}k$, this suggests that moving the near-wall nodes further from the wall decreases the predicted near-wall turbulent kinetic energy.

Figure 6.11: Friction Factor Sensitivity Study, $\gamma_p = 1.1$ Figure 6.12: Friction Factor Sensitivity Study, $\gamma_p = 1.375$

Figure 6.13: Friction Factor Sensitivity Study, $\gamma_p = 1.833$

Reducing the number of control volumes by 54% reduces the friction factor by a maximum of 3.0% for $\gamma_p = 1.1$ and a maximum of 3.25% for $\gamma_p = 1.833$. In general, the coarser meshes exhibited higher friction factors than the finer meshes.

Figures 6.14 through 6.16 compare the base case gap Stanton numbers with those obtained from the mesh size and near-wall node sensitivity studies.

The sensitivity of gap Stanton number to near-wall node placement was far greater than the sensitivity to mesh resolution. For the $\gamma_p = 1.375$ case, moving the near-wall nodes outside $y^+ > 100$ decreased the gap Stanton number by approximately 20%, while for $\gamma_p = 1.833$, St_g increased by 36%. In comparison, the change in St_g due to reducing the mesh resolution was, on average, less than a percent. The greater sensitivity of St_g in the $\gamma_p = 1.375$ and $\gamma_p = 1.833$ cases as compared to the $\gamma_p = 1.1$ case is attributed to the lower turbulent effective conductivities calculated for larger values of γ_p . An alteration of the near-wall turbulent kinetic energy production due to movement of the near-wall nodes causes a larger percentage change in Γ_{eff} for larger values of γ_p than for smaller.

The sensitivity studies of near-wall node placement and mesh resolution concludes St_g sensitivity to mesh resolution is much less than sensitivity to near-wall node placement. The sensitivity of friction factor to near-wall node placement is slightly less than

Figure 6.14: Gap Stanton Numbers Sensitivity Study, $\gamma_p = 1.1$ Figure 6.15: Gap Stanton Numbers Sensitivity Study, $\gamma_p = 1.375$

Figure 6.16: Gap Stanton Number Sensitivity Study, $\gamma_p = 1.833$

sensitivity to mesh resolution. Sensitivity to both parameters, however, is less than a few percent in the case of friction factor.

6.7.2 Inlet Turbulence Parameter Sensitivity

The inlet boundary condition for the turbulence model consisted of a specified turbulence intensity, T_u , of 5% and a turbulence length scale, L_ϵ , equal to the gap width. The sensitivity of the final results to selection these values was investigated.

Table 6.6 compares two code executions, with different inlet turbulence characteristics. The base case was duct 5 ($\gamma_p = 1.1$) with a Reynolds number of 3.44×10^4 .

The sensitivity of predicted quantities to the choice of inlet turbulence parameters is less than a fraction of a percent, with the friction factor exhibiting the largest sensitivity. If the inlet turbulence parameters are changed by a factor larger than that given in Table 6.6, the outlet quantities are expected to change very little given a long enough development length. In other words, choice in inlet turbulence parameters are expected to alter the development length rather than the values of the fully developed results.

Table 6.6: Sensitivity to Inlet Turbulence Parameters, $\gamma_p = 1.1$, $Re = 3.44 \times 10^4$

	Base Case $T_u = 0.05$ $L_\epsilon = 5 \times 10^{-3} m$	Sensitivity Case $T_u = 0.06$ $L_\epsilon = 7 \times 10^{-3} m$	Difference [%]
Friction factor	5.951×10^{-3}	5.923×10^{-3}	-0.47
$k^{3/2}/\epsilon$ in gap at outlet	$2.68394 \times 10^{-3} m$	$2.68390 \times 10^{-3} m$	-0.0015
$k^{3/2}/\epsilon$ at U_{max} at outlet	$6.9781 \times 10^{-3} m$	$6.9785 \times 10^{-3} m$	0.0057
Top subchannel T_b	966.3 K	967.6 K	0.13
Bottom subchannel T_b	324.36 K	324.42 K	0.02
St_g	7.282×10^{-4}	7.268×10^{-4}	-0.19

6.8 Summary

Analysis of the code predicted friction factors reveals a good agreement with both measured results and Cheng and Todreas' correlation. Turbulent interchange mixing, however, is underpredicted. The largest underprediction is observed for the tightest-packed rod case ($\gamma_p = 1.1$).

Owing to large scatter in Seale's gap Stanton measurement coupled with the poor St_g results predicted by the code, confirmation of Nikuradse's relationship between the friction factor and turbulent interchange mixing could not be confirmed.

Analysis of the turbulent eddy diffusivity field reveals a good agreement with experimental and analytical data. The isotropic eddy diffusivity model used in this investigation matched well with the radial component of Rehme's data. This is consistent with the observed good prediction of friction factor, and therefore average wall shear. A different value for the azimuthal component of eddy viscosity, however, is not calculated by the isotropic model used in this investigation. Because the azimuthal component has been measured to be up to 100 times larger than the radial component in the gap of tightly packed rods, the isotropic model underpredicts azimuthal diffusion momentum and heat in the gap. Underprediction of the azimuthal diffusion of momentum results in the observed underprediction of axial velocity in the gap. Underprediction of the azimuthal diffusion of heat results in the observed underprediction of turbulent interchange mixing and hence the large temperature gradients across the gap.

While some authors found an anisotropy distribution which yielded better turbulent mixing results, the nature of such distributions renders independent experimental confirmation of the distribution difficult. A turbulence model that models the various Reynolds stress terms independently is recommended, such as the algebraic stress model presented by Launder and Spalding [59]. The feasibility and limitations of using such a model should be explored.

Chapter 7

Closure

7.1 Summary and Conclusions

This objective of this research was to first understand the physical behaviour of coolant mixing within a nuclear fuel bundle and second to assess the applicability of a computational model of turbulent interchange mixing.

A mathematical model of steady, three-dimensional turbulent fluid flow was presented in conjunction with a numerical solution procedure based upon finite volumes. Turbulence was modeled using an isotropic, $k - \varepsilon$ eddy viscosity model. Turbulent heat transfer utilized a constant turbulent Prandtl number of 0.9.

Preliminary validation suggested the mathematical and numerical models adequately predicted the momentum, energy, and turbulence fields of simple flows in circular pipes. Laminar buoyancy-driven flow in a square cavity was similarly well predicted.

Turbulent interchange mixing between adiabatic rods was validated against an experiment performed by Seale [37]. Although the friction factor was predicted well, turbulent interchange mixing was underpredicted. The amount of underprediction was most pronounced for smaller pitch-to-diameter ratios (*i.e.* tighter packed rods).

Due to the underprediction in turbulent interchange mixing and the scatter in Seale's gap Stanton number results, the square-root relationship between St_g and friction factor could not be demonstrated satisfactorily.

Further analysis of the results revealed the isotropic turbulent eddy viscosity, μ_t , as calculated by the $k - \varepsilon$ model compares favourably with the radial component of turbulent eddy viscosity measured by Rehme [19]. This good agreement is attributed to the applicability of the law of the wall in rod bundle geometries coupled with the presence of turbulence equilibrium in the radial direction. The accurate friction factor

predictions are attributed to these accurate radial μ_t results.

Other experimental evidence suggests an azimuthal component of μ_t up to 100 times greater than the radial component. The observed underprediction of turbulent interchange mixing and axial velocity in the gap is attributed to this underprediction of the azimuthal component of μ_t .

7.2 Recommendations for Further Work

1. Mesh independent results were not demonstrated in this investigation (with a 54% reduction in nodes, the friction factor changed by 3% while the gap Stanton number changed by less than 1%). Therefore additional mesh refinement in the plane parallel to the flow axis is recommended. Such refinement, however, is not expected to improve the code predictions because the differences between the code and experiment are attributed to the mathematical, rather than numerical, model.
2. Because of its relatively direct measurement of turbulent interchange mixing, the experiment performed by Seale should continue to be used as a final validation dataset. In addition, the experimental apparatus provides for symmetry and other computational cost savings.
3. Instead of using an isotropic eddy viscosity turbulence model, a model capable of predicting at least azimuthal and radial variations in turbulent eddy viscosity should be used. An algebraic turbulent stress model is suggested because such a model represents a logical increase in complexity. A recommendation of a specific turbulence model, however, can not be made until the relative strengths and weaknesses of different algebraic turbulence models are reviewed.
4. The use of anisotropy functions to augment the azimuthal component of turbulent eddy viscosity (such as those used by Seale[11] and Yang and Chieng [61]) are not recommended because Seale observes experimental validation of such factors is difficult.

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Appendix A

Secondary Flows

Johnston [62] describes secondary flow as “a generic term used to denote the mean cross flow field characterized by the velocity components V and W that lie in a plane which is normal to the x , ‘main’, flow direction.” In particular, two types of secondary flow are described by Johnston: *secondary flow of the first kind* and *secondary flow of the second kind*.

Secondary flow of the first kind has two principle source mechanisms: lateral curvature of the main flow (such as flow through a bending pipe) and lateral wall motion (such as flow in a pipe rotating about its axis). Since these conditions do not normally exist within the core of a reactor, secondary flow of the first kind is not of interest in studies of rod bundles.

Secondary flow of the second kind, as identified by Prandtl, is generated by gradients of the Reynolds stresses. In other words, secondary flow of the second kind is entirely caused by turbulence. While secondary flows of the first kind are present in both laminar and turbulent regimes, flows of the second kind are only present in turbulent flows. Johnston points out that secondary flows of the second kind are important for slender shear flows along edges aligned with the flow or corners. A well-known example of this phenomenon is observation of small secondary flows in the corners of an axially-dominated rectangular duct flow. Secondary flow of the second kind is most certainly of interest in subchannel studies.

Since secondary flow of the second kind is turbulence-driven, clearly an equation involving either Reynolds stresses or turbulence parameters is required to describe these motions. Demuren and Rodi [63] provide such an equation by considering the time-averaged stream-wise vorticity in the axial direction, Ω_1 . The time-averaged vorticity,

Ω_1 , is given by the following.

$$\Omega_1 = \frac{\partial U_2}{\partial x_2} - \frac{\partial U_3}{\partial x_3} \quad (\text{A.1})$$

The equation for secondary flow of the second kind, in terms of the vorticity, is given by the following [63].

$$\begin{aligned} & \overbrace{U_2 \frac{\partial \Omega_1}{\partial x_2} + U_3 \frac{\partial \Omega_1}{\partial x_3}}^{\text{I}} \\ &= \underbrace{\frac{\partial^2}{\partial x_2 \partial x_3} (\overline{u_3^2} - \overline{u_2^2})}_{\text{II}} - \underbrace{\left(\frac{\partial^2}{\partial x_3^2} - \frac{\partial^2}{\partial x_2^2} \right) \overline{u_2 u_3}}_{\text{III}} + \underbrace{\nu \left(\frac{\partial^2 \Omega_1}{\partial x_2^2} + \frac{\partial^2 \Omega_1}{\partial x_3^2} \right)}_{\text{IV}} \end{aligned} \quad (\text{A.2})$$

Term I represents the convection of vorticity, Term II represents a vorticity source, Term III a vorticity sink, and Term IV the viscous dissipation of vorticity. Under conditions of laminar flow, Terms II and III are, of course, zero (there are no turbulent stresses). Hence, Terms II and III alone are responsible for the generation of secondary flow of the second kind. Schetz and Fuhs [64] point out that for fully developed flow in axisymmetric ducts, symmetry conditions force Terms II and III to zero, thereby implying that secondary flow of the second kind is not present in turbulent flow in such ducts¹. Further, Schetz and Fuhs point out that in the absence of Terms II and III (which are sources and sinks) all that remains is Term IV, which is dissipative. In other words, eventually the viscous dissipation of vorticity will yield an equation as shown.

$$\begin{aligned} & \underbrace{U_2 \frac{\partial \Omega_1}{\partial x_2} + U_3 \frac{\partial \Omega_1}{\partial x_3}}_{\text{I}} = \underbrace{\nu \left(\frac{\partial^2 \Omega_1}{\partial x_2^2} + \frac{\partial^2 \Omega_1}{\partial x_3^2} \right)}_{\text{IV}} \\ & \qquad \qquad \qquad \rightarrow 0 \end{aligned} \quad (\text{A.3})$$

Hence, as the viscous dissipation of vorticity goes to zero, so too does the convection of vorticity, and secondary flow is not generated. This is indeed the case in laminar flow.

Demuren and Rodi cite the experimental work of Gessner and Jones who indicate that for axial flow in a rectangular duct, the turbulence terms in Equation (A.2) (*i.e.* II and III) are two orders of magnitude greater than the convection term, I, while the viscous dissipation term is negligible except in close proximity to the wall. In fact, since Terms II and III are of opposite sign, it is the slight *difference* between these terms which balance the convection of vorticity under equilibrium conditions. This presents an interesting challenge to the modeler: the gradients of both $\overline{u_3^2} - \overline{u_2^2}$ and $\overline{u_2 u_3}$ must be determined

¹Note that Equation (5.45) on page 498 of Schetz and Fuhs [64] appears incorrect, as Term II contains a total derivative of x_1 rather than a partial derivative of x_3 .

accurately enough such that the difference between the two (which is of the same order as Term I and therefore two orders of magnitude less than either Term II or III) balances properly with the convection term. Many authors, including Rodi [65] and Hanjalić [66] agree that eddy viscosity models, such as the $k - \epsilon$ model, cannot meet this requirement.

Appendix B

Evaluation of Diffusion and Advection Terms Model

B.1 Evaluation of Diffusion Term

The diffusion term is evaluated using a finite element approach. Recall that integration points are interior points to finite elements; each non-surface finite element has twelve integration points within it. To evaluate an integration point, shape functions, N_n , are used to sum the values of scalar values at nodal points, φ_n .

$$\varphi_{ip} = \sum_n N_n|_{ip} \varphi_n \quad (\text{B.1})$$

Using this, the gradients of scalars at diffusion points can be written as gradients of shape functions.

$$\left. \frac{\partial \varphi}{\partial x} \right|_{ip} = \sum_n \left. \frac{\partial N_n}{\partial x} \right|_{ip} \varphi_n \quad (\text{B.2})$$

The shape functions are chosen such that for node i , $N_i = 1$ and $N_j = 0$ for all $j \neq i$ and the sum of all shape functions at any point equals one.

As per the standard finite element approach, the derivatives of the shape functions in global coordinates, x_i , are transformed into derivatives of local or intrinsic coordinates, ξ_i , by means of the Jacobian transformation matrix.

$$\begin{pmatrix} \frac{\partial N}{\partial x_1} \\ \frac{\partial N}{\partial x_2} \\ \frac{\partial N}{\partial x_3} \end{pmatrix} = \begin{pmatrix} \frac{\partial x_1}{\partial \xi_1} & \frac{\partial x_2}{\partial \xi_1} & \frac{\partial x_3}{\partial \xi_1} \\ \frac{\partial x_1}{\partial \xi_2} & \frac{\partial x_2}{\partial \xi_2} & \frac{\partial x_3}{\partial \xi_2} \\ \frac{\partial x_1}{\partial \xi_3} & \frac{\partial x_2}{\partial \xi_3} & \frac{\partial x_3}{\partial \xi_3} \end{pmatrix}^{-1} \begin{pmatrix} \frac{\partial N}{\partial \xi_1} \\ \frac{\partial N}{\partial \xi_2} \\ \frac{\partial N}{\partial \xi_3} \end{pmatrix} \quad (\text{B.3})$$

Evaluation of gradients at integration points by means of linear shape functions is second order accurate within orthogonal elements but only first order accurate within

non-orthogonal elements [67]. However, as the aspect ratio becomes large or the element becomes skewed, the evaluation of gradients becomes poor. As such, poor convergence and/or oscillatory solutions may be observed.

A means of improving solution robustness at the expense of solution accuracy is to evaluate the shape function derivatives at the locations where the integration point surfaces intersect the finite element edge. Such an approach, called ‘linear-linear’ evaluation, is first-order accurate for both orthogonal and non-orthogonal grids. For an orthogonal grid, poor convergence and oscillatory behaviour is never experienced [67], which is very important in resolving boundary layers.

B.2 Evaluation of Advection Term

Unfortunately, evaluation of the transported scalar, φ , at the integration points is not as straightforward as for the diffusion terms. While the diffusion terms are elliptic, the advection terms are hyperbolic. Shape functions are elliptic, as all neighbouring nodes equally influence the evaluated value. Using elliptical approaches yields non-physical results as explained by considering a flow moving left-to-right. Blue dye is inserted into the flow at a particular location, and red dye is inserted downstream. The question to ask is: what is the colour of the dye at the midpoint between the two insertion locations? Intuition indicates the dye should be blue, as the flow carries the blue dye downstream and red dye is unable to influence the fluid colour upstream of its insertion location. As the flow slows, however, the red dye is increasingly able to diffuse backward against the flow. At the limit where the flow approaches zero, both the blue and red dyes are transported by diffusion alone, hence the midpoint between the two insertion locations will be equally influenced by both dyes (and the fluid, therefore, a combination of red and blue).

This velocity-based dependence of advection’s influence on an integration point’s value requires careful treatment of the advection term.

A simple, but first-order accurate advection model is the upstream differencing scheme. This scheme assigns the value of φ at an integration point to that of the node immediately upstream of the integration point. Consider the one-dimensional control volume in Figure B.1. For a left-to-right flow, upwinding implies the following φ value for the integration point, e .

$$\varphi_e = \varphi_i \tag{B.4}$$

For high-speed flows parallel to the grid, this is a very reasonable assumption. However,

Figure B.1: One Dimensional Control Volume

for lower speed or skewed flows, more accurate models are available.

Correction terms are introduced to the upstream differencing scheme to capture the physical dependence of an integration point on neighbouring nodes as the flow velocity changes.

$$\varphi_e = \varphi_i + \frac{\Delta x}{2} \left(\frac{\partial \varphi}{\partial x} \right)_e \quad (\text{B.5})$$

One method of evaluating $(\partial \varphi / \partial x)_e$ is to use the first term of the Taylor expansion.

$$\frac{\partial \varphi}{\partial x} \approx \frac{\varphi_{i+1} - \varphi_i}{\Delta x} \quad (\text{B.6})$$

Substitution of this term into Equation B.5 results in the following expression.

$$\varphi_e = \frac{1}{2} (\varphi_i + \varphi_{i+1}) \quad (\text{B.7})$$

This central difference scheme, unfortunately, does not yield a physically realistic dependence of φ_e on its neighbouring nodes. Both the upstream and downstream nodes influence the value of φ_e equally.

An alternate approach is to combine the central difference scheme with the purely upwinded scheme. Weighting or blending functions are used to control the degree of upwind and central difference contribution to the advection term [55]. The blending function uses the grid Peclet number, $Pe_{\Delta x}$.

$$\varphi_e = \frac{Pe_{\Delta x}^2}{5 + Pe_{\Delta x}^2} \frac{1}{2} (\varphi_i + \varphi_{i+1}) + \left(1 - \frac{Pe_{\Delta x}^2}{5 + Pe_{\Delta x}^2} \right) \varphi_i \quad (\text{B.8})$$

The grid Peclet number is given by the following.

$$Pe_{\Delta x} = \frac{\rho c_p u_i \Delta x}{\Gamma} \quad (\text{B.9})$$

Another approach, the second order upwind differencing scheme [68, 69] evaluates the derivative $(\partial\varphi/\partial x)_e$ using the fully upwinded values. However, a negative coefficient on φ_{i-1} is created, which can lead to convergence difficulties [53].

The QUICK method [70] combines central differencing with second order upwind differencing. However, non-physical downstream influences are introduced.

Physical advection correction (PAC) schemes provide a correction for the upwinded value by discretizing the derivative $(\partial u/\partial x)_e$ using equations which emulate the physical processes inherent in advection. Thus, the correction to φ_e correctly reflects the interactions of advection, diffusion, and source terms.

Consider the steady state transport equation (Equation 3.56). Writing in non-conservative form (*i.e.* applying the continuity equation) the following is obtained.

$$\rho u_j \frac{\partial \varphi}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \varphi}{\partial x_j} \right) + S_\varphi \quad (\text{B.10})$$

Rearranging, and mixing Einstein notation with Cartesian, one of the advective derivatives can be expressed in terms of the remainder.

$$\frac{\partial \varphi}{\partial x} = \frac{1}{\rho u} \left[S_\varphi + \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \varphi}{\partial x_j} \right) - \rho v \frac{\partial \varphi}{\partial y} - \rho w \frac{\partial \varphi}{\partial z} \right] \quad (\text{B.11})$$

The above equation is used to evaluate $(\partial\varphi/\partial x)_e$ in Equation B.5.

$$\varphi_e = \varphi_i + \frac{\Delta x}{2\rho u} \left[S_\varphi + \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \varphi}{\partial x_j} \right) - \underbrace{\rho v \frac{\partial \varphi}{\partial y}}_{\text{I}} - \underbrace{\rho w \frac{\partial \varphi}{\partial z}}_{\text{II}} \right] \quad (\text{B.12})$$

Discretization of terms I and II, however, can lead to non-physical ‘wiggles’ in φ , particularly in situations where advection dominates.

The skew upstream differenceing scheme (SUDS) corrects this problem by removing the dependence of the PAC equation on advection. Instead of considering the transport equation in Cartesian coordinates, SUDS solves the advection equation along a streamline following the flow. The velocity along the streamline is given by the vector $\vec{V}$, and s is the parametric position on the streamline.

$$\begin{aligned} \rho |\vec{V}| \frac{\partial \varphi}{\partial s} &= \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \varphi}{\partial x_j} \right) + S_\varphi \\ \frac{\partial \varphi}{\partial s} &= \frac{1}{\rho |\vec{V}|} \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \varphi}{\partial x_j} \right) + S_\varphi \end{aligned} \quad (\text{B.13})$$

The upwinded point which is corrected is no longer i but rather some point P on the streamline (Figure B.2). The distance from the integration point e to P is given by l .

$$\varphi_e = \varphi_P + l \frac{\partial \varphi}{\partial s}$$

Figure B.2: Skewed upwinding in two dimensions

$$= \varphi_P + l \frac{1}{\rho |\vec{V}|} \underbrace{\frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \varphi}{\partial x_j} \right)}_I + S_\varphi \quad (\text{B.14})$$

The value of φ_P is evaluated using a mass weighted approach. φ_P is determined by averaging the surrounding nodal values weighted by the mass flow through each control volume face surrounding P . This is first-order accurate, but eliminates the non-physical ‘wiggles’ observed in the solution of φ [67].

Evaluation of term I in Equation B.14 is facilitated by the observation that all of the elements in term I are already calculated and available at nodal points. However, for use in the PAC scheme, these values are required at integration points. This is accomplished by using the harmonic mean of term I at surrounding nodal points. The use of the harmonic mean avoids over- and underpredictions at discontinuities (*i.e.* shock boundaries).

The PAC terms are implemented explicitly, that is, lagged in the equations. This can lead to oscillations unless underrelaxation of the change in PAC terms is introduced.

Appendix C

The Colocated Grid

C.1 Pressure / Velocity Coupling and Grid Colocation

A difficulty of solving the governing equations is the weak of coupling between the pressure and velocity fields. The equation for pressure (the continuity equation) does not explicitly contain pressure but rather contains the *influence* of pressure on the velocity field.

Consider the one dimensional conservation of mass over a one-dimensional control volume (Figure B.1).

$$\rho A u_e - \rho A u_w = 0 \quad (\text{C.1})$$

The variables u_e and u_w represent the velocities at the east and west faces of the control volume, respectively. One approach to estimating u_e and u_w is to use the average of the neighbouring nodal velocities.

$$\begin{aligned} u_w &= \frac{1}{2} (u_{i-1} + u_i) \\ u_e &= \frac{1}{2} (u_i + u_{i+1}) \end{aligned} \quad (\text{C.2})$$

Substitution of the above equation into Equation (C.1) yields an interesting result.

$$u_{i+1} - u_{i-1} = 0 \quad (\text{C.3})$$

The velocity field at i (*i.e.* u_i) does not appear in the continuity equation. Next consider a simple form of the momentum equation over the same control volume.

$$\rho A u_i (u_{i+1} - u_{i-1}) + \frac{A}{2} (p_{i+1} - p_{i-1}) = 0 \quad (\text{C.4})$$

However, as $u_{i+1} - u_{i-1} = 0$, the momentum equation above, implies that $p_{i-1} - p_{i+1} = 0$. Neither the velocity nor the pressure at point i appear in the equation.

This lack of coupling can give rise to physically meaningless results. Patankar [53] discusses how pressure ‘checkerboarding’ can occur when pressure and velocity nodes are *colocated* or placed at the same location. A common remedy is to stagger the pressure (and therefore mass) grid with respect to the velocity grid. As such, pressure (and mass) are calculated at nodal points, while velocities are calculated at integration points.

A drawback of grid staggering is the added complications which arise on the boundaries of Cartesian grids. In addition, the presence of effectively two different grids requires additional calculations of various parameters (such as volume, face areas, *etc.*) which are required only once with a colocated grid.

The solution is to solve the discretized equations in a manner which does not suffer from pressure/velocity decoupling and subsequent ‘checkerboarding’ of the pressure field. This is accomplished by splitting the velocity into two components, one associated with the pressure gradient, and one independent of the gradient.

Consider the equation for conservation of momentum over a one-dimensional control volume around node i .

$$(A_p)_i u_i = \left(\sum_{nb} A_{nb} u_{nb} \right)_i - V \left(\frac{\partial p}{\partial x} \right)_i + b_i \quad (C.5)$$

Dividing through by area $(A_p)_i$, we obtain an expression for the velocity at point i as a sum of two main velocity components, I and II.

$$u_i = \underbrace{\frac{1}{(A_p)_i} \left[\left(\sum_{nb} A_{nb} u_{nb} \right)_i + b_i \right]}_I - \underbrace{\frac{V}{(A_p)_i} \left(\frac{\partial p}{\partial x} \right)_i}_{II} \quad (C.6)$$

Component I is a velocity independent of the pressure gradient. This pressure-independent velocity is denoted as $\hat{u}_i$.

$$\hat{u}_i = \underbrace{\frac{1}{(A_p)_i} \left[\left(\sum_{nb} A_{nb} u_{nb} \right)_i + b_i \right]}_I \quad (C.7)$$

Component II is the influence of a pressure gradient on the velocity at point i . The coupling between the u_i and the pressure gradient is denoted as d_i . This represents an effective distance over which the pressure gradient acts¹.

$$d_i = -\frac{V}{(A_p)_i} \quad (C.8)$$

¹For constant area control volumes, d_i represents the width of the control volume. If the control volume is narrower at the nodal point than at the ends, d_i is longer than the control volume width.

Making these substitutions, the momentum conservation equation for the control volume can be written in terms of a pressure gradient and a velocity independent of pressure gradient.

$$u_i = \underbrace{\hat{u}_i}_I + \underbrace{d_i \left(\frac{\partial p}{\partial x} \right)_i}_{II} \quad (C.9)$$

Rearranging, an equation for the pressure gradient independent velocity, $\hat{u}_i$, is obtained.

$$\hat{u}_i = u_i - d_i \left(\frac{\partial p}{\partial x} \right)_i \quad (C.10)$$

Now consider the same equation written for an integration point (*i.e.* on the boundary between control volumes) to the 'east' of the centre node.

$$u_e = d_e \left(\frac{\partial p}{\partial x} \right)_e + \hat{u}_e \quad (C.11)$$

The east velocity independent of pressure gradient can be approximated as the average of its neighbour nodal velocities.

$$\hat{u}_e = \frac{1}{2} (\hat{u}_i + \hat{u}_{i+1}) \quad (C.12)$$

Similarly, the pressure gradient characteristic distance can be expressed as the average of the neighbouring values.

$$d_e = \frac{1}{2} (d_i + d_{i+1}) \quad (C.13)$$

Hence, the equation for the east face velocity is written as shown.

$$u_e = \frac{1}{2} (\hat{u}_i + \hat{u}_{i+1}) + \frac{1}{2} (d_i + d_{i+1}) \left(\frac{\partial p}{\partial x} \right)_e \quad (C.14)$$

Substitution of Equation (C.10) into the above equation yields an expression for the velocity at the east face in terms of nodal, (rather than pressure gradient independent) velocities.

$$u_e = \frac{1}{2} (u_i + u_{i+1}) + \frac{1}{2} (d_i + d_{i+1}) \left(\frac{\partial p}{\partial x} \right)_e - \frac{1}{2} \left[d_i \left(\frac{\partial p}{\partial x} \right)_i + d_{i+1} \left(\frac{\partial p}{\partial x} \right)_{i+1} \right] \quad (C.15)$$

Rearranging, the following is obtained.

$$\begin{aligned} u_e = & \frac{1}{2} (u_i + u_{i+1}) + \frac{1}{2} (d_i + d_{i+1}) \left\{ \left(\frac{\partial p}{\partial x} \right)_e - \frac{1}{2} \left[\left(\frac{\partial p}{\partial x} \right)_i + \left(\frac{\partial p}{\partial x} \right)_{i+1} \right] \right\} \\ & - \frac{1}{4} (d_i - d_{i+1}) \left[\left(\frac{\partial p}{\partial x} \right)_i - \left(\frac{\partial p}{\partial x} \right)_{i+1} \right] \end{aligned} \quad (C.16)$$

Given that as the control volumes decrease in size, $d_i \rightarrow d_{i+1}$ and $(\partial p/\partial x)_i \rightarrow (\partial p/\partial x)_{i+1}$, the second line of the preceding equation can be considered negligible. Thus, the velocity at the east face can be approximated as follows.

$$u_e \approx \frac{1}{2} (u_i + u_{i+1}) + \frac{1}{2} (d_i + d_{i+1}) \left\{ \left(\frac{\partial p}{\partial x} \right)_e - \frac{1}{2} \left[\left(\frac{\partial p}{\partial x} \right)_i + \left(\frac{\partial p}{\partial x} \right)_{i+1} \right] \right\} \quad (C.17)$$

The reason for performing the rearrangement to obtain the above approximation will be clear momentarily.

A similar equation can be written for the velocity at the west face.

$$u_w \approx \frac{1}{2} (u_{i-1} + u_i) + \frac{1}{2} (d_{i-1} + d_i) \left\{ \left(\frac{\partial p}{\partial x} \right)_w - \frac{1}{2} \left[\left(\frac{\partial p}{\partial x} \right)_{i-1} + \left(\frac{\partial p}{\partial x} \right)_i \right] \right\} \quad (C.18)$$

Substitution of these equations for u_e and u_w into Equation (C.1) provides an expression for mass conservation which explicitly includes the velocities and pressure gradients at the nodal points ($i-1, i, i+1$) and integration points (w, e). The gradients at the integration points can be linearized using nodal pressures.

$$\begin{aligned} \left(\frac{\partial p}{\partial x} \right)_e &= \frac{p_{i+1} - p_i}{x_{i+1} - x_i} \\ \left(\frac{\partial p}{\partial x} \right)_w &= \frac{p_i - p_{i-1}}{x_i - x_{i-1}} \end{aligned} \quad (C.19)$$

For the simplified case of one-dimensional flow in a constant area duct, the mass conservation equation is written as shown.

$$u_{i+1} - u_{i-1} + \frac{1}{\rho u_i} (-p_{i-2} + 4p_{i-1} - 6p_i + 4p_{i+1} - p_{i+2}) = 0 \quad (C.20)$$

If the rearrangement performed in Equation C.16 were not made, subtracting u_w from u_e would cause p_i , the pressure at node i , to disappear. By performing the rearrangement and using the approximate expressions for u_w and u_e , pressure/velocity decoupling and subsequent “checkerboarding” is avoided.

It is interesting to compare the Equation (C.20) to Equation (C.3). The introduction of nodal pressure terms into the momentum permits the use of colocated pressure and velocity nodes, thereby removing the complicated requirements of staggered grids. Local underestimates or overestimates of pressure and velocity in regions of large gradients (*i.e.* near a shock) are not precluded, however. This localized behaviour can be resolved with appropriate grid refinement. So such gradients are expected in the current investigation.

C.2 Transient Multidimensional Representation

Expressing pressure/velocity coupling for a transient problem in two or more dimensions is somewhat more complicated than that of the one dimensional case presented in the previous section.

Consider the nodal momentum conservation equation for the u component of momentum over a domain of two or more dimensions.

$$\left(A_p + \rho \frac{V}{\Delta t}\right)_{NP} u_{NP} = \left(\sum_{nb} A_{nb} u_{nb}\right)_{NP} + b_{NP} - V_{NP} \left(\frac{\partial p}{\partial x}\right)_{NP} + \left(\rho \frac{V}{\Delta t}\right)_{NP} u_{NP}^0 \quad (C.21)$$

The subscript NP indicates the coefficients are associated with a particular nodal point, while nb represents the neighbouring nodal points. The area A is the control volume area perpendicular to the x direction (since the u momentum equation is under consideration). Dividing through by the area, A_p , the following is obtained.

$$\left(1 - \frac{\rho d_{NP}}{\Delta t}\right) u_{NP} = \hat{u}_{NP} + d_{NP} \left(\frac{\partial p}{\partial x}\right)_{NP} - \frac{\rho d_{NP}}{\Delta t} u_{NP}^0 \quad (C.22)$$

where:

$$\begin{aligned} d_{NP} &= -\frac{V_{NP}}{A_p} \\ \hat{u}_{NP} &= \frac{[(\sum_{nb} A_{nb} u_{nb})_{NP} + b_{NP}]}{A_p} \end{aligned}$$

Given an integration point ip (*i.e.* e in Figure B.1), consider the following form of the x momentum equation.

$$\left(1 - \frac{\rho d_{ip}}{\Delta t}\right) u_{ip} = \hat{u}_{ip} + d_{ip} \left(\frac{\partial p}{\partial x}\right)_{ip} - \frac{\rho d_{ip}}{\Delta t} u_{ip}^0 \quad (C.23)$$

where:

$$\begin{aligned} d_{ip} &= \text{an average of } d_{NP}; \text{ the surrounding nodal values of } d \\ \hat{u}_{ip} &= \text{an average of } \hat{u}_{NP}; \text{ the surrounding nodal values of the} \\ &\quad \text{velocity independent of the pressure gradient} \\ \left(\frac{\partial p}{\partial x}\right) &= \text{evaluated using the nodal pressures around the} \\ &\quad \text{integration point} \\ u_{ip}^0 &= \text{value of } u_{ip} \text{ from previous time step} \end{aligned}$$

The average of the surrounding nodal values of $\hat{u}_{NP}$, $\hat{u}_{ip}$, is determined by rearranging Equation (C.22) in terms of $\hat{u}_{NP}$ and averaging over the neighbouring nodal points.

$$\hat{u}_{ip} = \frac{\sum_{NP} \left(1 - \frac{\rho d_{NP}}{\Delta t}\right) u_{NP} - d_{NP} \left(\frac{\partial p}{\partial x}\right)_{NP} + \frac{\rho d_{NP}}{\Delta t} u_{NP}^0}{n_{NP}} \quad (C.24)$$

where n_{NP} is the number of neighbouring nodal points. For convenience, an overbar can be used to represent the average value.

$$\hat{u}_{ip} = \overline{\left(1 - \frac{\rho d_{NP}}{\Delta t}\right) u_{NP} - d_{NP} \left(\frac{\partial p}{\partial x}\right)_{NP} + \frac{\rho d_{NP}}{\Delta t} u_{NP}^0} \quad (C.25)$$

Substitution of the above equation into Equation (C.23) yields the following.

$$\begin{aligned} \left(1 - \frac{\rho d_{ip}}{\Delta t}\right) u_{ip} = & \overline{\left(1 - \frac{\rho d_{NP}}{\Delta t}\right) u_{NP} - d_{NP} \left(\frac{\partial p}{\partial x}\right)_{NP} + \frac{\rho d_{NP}}{\Delta t} u_{NP}^0} \\ & + d_{ip} \left(\frac{\partial p}{\partial x}\right)_{ip} - \frac{\rho d_{ip}}{\Delta t} u_{ip}^0 \end{aligned} \quad (C.26)$$

The above is simplified by making the following approximation.

$$\overline{d_{NP} \left(\frac{\partial p}{\partial x}\right)_{NP}} \approx d_{ip} \left(\frac{\partial p}{\partial x}\right)_{NP} \quad (C.27)$$

Using the above approximation and dividing through by $1 - \frac{\rho d_{ip}}{\Delta t}$, an expression for the velocity at an integration point is obtained.

$$u_{ip} = \bar{u}_{NP} + f \left[\left(\frac{\partial p}{\partial x}\right)_{ip} - \left(\frac{\partial p}{\partial x}\right)_{NP} \right] - \frac{\rho f}{\Delta t} (u_{ip}^0 - \bar{u}_{NP}^0) \quad (C.28)$$

where:

$$\begin{aligned} \bar{u}_{NP} &= \text{average of surrounding nodal velocities} \\ f &= \frac{d_{ip}}{1 - \frac{\rho d_{ip}}{\Delta t}} \\ \left(\frac{\partial p}{\partial x}\right)_{NP} &= \text{average of surrounding pressure gradients} \end{aligned} \quad (C.29)$$

The characteristic distance over which pressure acts at the integration point, d_{ip} , was evaluated in the one dimensional case by dividing the volume by the cross-sectional area. In two or more dimensions, d_{ip} is expressed by the following.

$$d_{ip} = - \frac{V_{fe}}{\sum_{fe} |\dot{m}_{ip}| + 8(\mu + \mu_t) \frac{|A_{ip}|}{\Delta_{ip}}} \quad (C.30)$$

Note that the volume of a *finite element* is used when defining d_{ip} for an integration point. $\sum_{fe} |\dot{m}_{ip}|$ is the sum of the absolute values of mass flow through all integration points within the finite volume. The quantity $\frac{|A_{ip}|}{\Delta_{ip}}$ is the cross-sectional area of the finite volume at the integration point perpendicular to the velocity vector divided by the distance across the element, through the integration point and normal to the plane of A_{ip} .

C.3 Order of Convergence and Stability

Taylor series expansion of $\hat{u}_p$ and $\hat{u}_e$ around point e yields the following:

$$\hat{u}_e = u_e + \left(\frac{\Delta x^2}{8} \right) \frac{\partial^2 u}{\partial x^2} + f \left\{ \frac{\Delta x^2}{8} \frac{\partial^3 P}{\partial x^3} \Big|_e \right\} - \frac{\rho f}{\Delta t} \left\{ \frac{\Delta x^2}{8} \frac{\partial^2 u^0}{\partial x^2} \right\} \quad (\text{C.31})$$

Thus, as the grid is refined, $\hat{u}_e \rightarrow u_e$ with order $(\Delta x)^2$. In other words, the colocated velocity approaches the ‘true’ velocity with second-order convergence.

Under steady-state conditions, $\hat{u}_e$ can also be shown to be independent of choice of timestep, Δt . At steady state, $\hat{u}_e = \hat{u}_e^0$, $u_i = u_i^0$ and $u_{i+1} = u_{i+1}^0$. Therefore,

$$\hat{u}_e^0 = \frac{1}{2} (u_{i+1}^0 + u_i^0) - \frac{\rho f}{\Delta t} \left[u_e^0 - \frac{1}{2} (u_{i+1}^0 + u_i^0) \right] - f \left[\frac{\partial P}{\partial x} \Big|_e - \frac{1}{2} \left(\frac{\partial P}{\partial x} \Big|_{i+1} + \frac{\partial P}{\partial x} \Big|_i \right) \right] \quad (\text{C.32})$$

Rearranging,

$$\hat{u}_e^0 = \frac{1}{2} (u_{i+1}^0 + u_i^0) - \underbrace{\frac{f}{1 + \frac{\rho f}{\Delta t}}}_{\text{I}} \left[\frac{\partial P}{\partial x} \Big|_e - \frac{1}{2} \left(\frac{\partial P}{\partial x} \Big|_{i+1} + \frac{\partial P}{\partial x} \Big|_i \right) \right] \quad (\text{C.33})$$

Term I can be rewritten as follows:

$$\begin{aligned} \frac{f}{1 + \frac{\rho f}{\Delta t}} &= \frac{d_e}{1 - \frac{\rho d_e}{\Delta t}} \frac{1}{1 + \frac{\rho}{\Delta t} \left(\frac{d_e}{1 - \frac{\rho d_e}{\Delta t}} \right)} \\ &= d_e \end{aligned} \quad (\text{C.34})$$

Thus,

$$\hat{u}_e^0 = \frac{1}{2} (u_{i+1}^0 + u_i^0) - d_e \left[\frac{\partial P}{\partial x} \Big|_e - \frac{1}{2} \left(\frac{\partial P}{\partial x} \Big|_{i+1} + \frac{\partial P}{\partial x} \Big|_i \right) \right] \quad (\text{C.35})$$

The time step, Δt , disappears from the expression for $\hat{u}_e^0$. Therefore the process of grid collocation does not introduce additional time step restrictions.

Appendix D

Convergence Behaviour of Point Solvers

Consider a one-dimensional domain Ω . After the m^{th} iteration of a system of discrete equations over the domain, an error value, $\Phi^m(x_i)$ exists at each discrete point, x_i , in Ω . Consider the Fourier representation of the error function over the length, L , of the domain after the m^{th} iteration.

$$\Phi^m(x) = \varphi(x) - \varphi^m(x) = \sum_{k=1}^N A_k^m e^{i\pi x k/L} \quad (D.1)$$

Note that at each nodal point, $i = \{1, \dots, N\}$, the error value is $\Phi^m(x_i)$, while in between, the error is approximated by the Fourier series. The variable k represents a *wavenumber* for the discrete Fourier solution, and ranges from $k = 1$ to $k = N$ where N is the number of equations solved. The component of Φ^m given by $k = N$ represents the highest frequency component of the error which can be determined using the N nodes in the domain.

The constant A_k^m represents the amplitude of each frequency component of the error. If a point solver, such as Gauss-Seidel, is converging quickly on each iteration, the ratio of A_k^{m+1} to A_k^m will be small. That is, on each successive iteration, the amplitude of the error function decreases.

Consider the form of a one-dimensional Gauss-Seidel solver.

$$a_P \varphi_P^{m+1} = a_w \varphi_W^{m+1} + a_e \varphi_E^m + b \quad (D.2)$$

The exact solution is provided by the following.

$$a_P \varphi_P = a_w \varphi_W + a_e \varphi_E + b \quad (D.3)$$

Subtracting Equation (D.2) from Equation (D.3), and substituting the definition of the error function, $\Phi^m(x) = \varphi(x) - \varphi^m(x)$, an equation for the error is obtained, assuming a uniform grid.

$$a_P \Phi^{m+1}(x_P) = a_W \Phi^{m+1}(x_P - \Delta x) + a_E \Phi^m(x_P + \Delta x) \quad (D.4)$$

Substituting the discrete Fourier form of the error, Equation (D.1), into the above equation yields the following.

$$\begin{aligned} a_P \sum_{k=1}^N A_k^{m+1} e^{i\pi x_P k/L} = \\ a_W \sum_{k=1}^N A_k^{m+1} e^{i\pi(x_P - \Delta x)k/L} + a_E \sum_{k=1}^N A_k^m e^{i\pi(x_P + \Delta x)k/L} \end{aligned} \quad (D.5)$$

Rearranging, we obtain the following.

$$\begin{aligned} \sum_{k=1}^N A_k^{m+1} e^{i\pi x_P k/L} (a_P - a_W e^{-i\pi \Delta x k/L}) = \\ \sum_{k=1}^N A_k^m e^{i\pi x_P k/L} (a_E e^{i\pi \Delta x k/L}) \end{aligned} \quad (D.6)$$

The convergence behaviour of the solver is determined by exploring the ratio of the A_k terms after each iteration. If the A_k term is smaller after each iteration, the error is decreasing. The smaller the ratio A_k^{m+1}/A_k^m , the faster the convergence. From Equation (D.6), the absolute value of the ratio of successive values of A_k is obtained.

$$\left| \frac{A_k^{m+1}}{A_k^m} \right| = \left| \frac{a_E e^{i\pi \Delta x k/L}}{a_P - a_W e^{-i\pi \Delta x k/L}} \right| \quad (D.7)$$

Converting to trigonometric form, and assuming a uniform grid with N control volumes (hence $\Delta x = L/N$), we obtain the following.

$$\left| \frac{A_k^{m+1}}{A_k^m} \right| = \left| \frac{a_E \cos(\pi k/N) + i a_E \sin(\pi k/N)}{a_P - a_W \cos(\pi k/N) + i a_W \sin(\pi k/N)} \right| \quad (D.8)$$

Consider a small wavenumber, $k = 1$. Assuming a large N , the cosine terms will be approximately equal to one, while the sine terms will be approximately equal to zero. Hence, for small wavenumbers, we obtain the following (assuming $a_W < a_P$ and all coefficients are positive, as required for conservation and stability [53]).

$$\begin{aligned} \left| \frac{A_1^{m+1}}{A_1^m} \right| &= \left| \frac{a_E}{a_P - a_W} \right| \\ &= \frac{a_E}{a_P - a_W} \end{aligned} \quad (D.9)$$

Now consider a large wavenumber, $k = N$. The cosine terms will be approximately equal to -1 (as $\cos(\pi) = -1$), and the sine terms will be again approximately zero. Thus, we obtain the following.

$$\begin{aligned} \left| \frac{A_N^{m+1}}{A_N^m} \right| &= \left| \frac{-a_E}{a_P + a_W} \right| \\ &= \frac{a_E}{a_P + a_W} \end{aligned} \tag{D.10}$$

Comparing Equation (D.9) to (D.10) we observe that the convergence ratio for large wavenumbers is smaller than that of small wavenumbers. Hence, we conclude that Gauss-Seidel solvers have the property that high-frequency components of the error (corresponding to large wavenumbers) ‘disappear’ faster than low-frequency components.

This ability of Gauss-Seidel solvers to remove high-frequency error components faster than low-frequency errors is the principle behind multigrid solution methods (Appendix E).

Appendix E

Multigrid

Since Gauss-Seidel point-solvers have the property that high-frequency errors are removed from the solution faster than low-frequency errors (Appendix D), it would be beneficial if error components could be as high frequency as possible.

The principle of multigridding is to translate the errors in a particular solution iteration onto a coarser grid thereby effectively increasing the frequency of the error component. A correction to the solution can be solved for on an even coarser grid, and so forth until a maximum grid coarseness is obtained. On the coarsest grid, the lowest frequency errors of the *original grid* are being solved, yet they appear to the Gauss-Seidel solver as high-frequency errors.

In the case of a finite volume method, the algebraic equations being solved by the Gauss-Seidel solver are conservation equations, hence errors in the solutions represent flux imbalances at control volume faces. The *additive correction multigrid* (ACM) method employed by TASCflow strives to sum the flux imbalances over a coarser block of neighbouring control volumes and equate this sum to zero. Consider the discrete form of a particular scalar equation defined at a fine control volume i .

$$a_i^p \varphi_i + \sum_{nb} a_i^{nb} \varphi_{nb} = b_i \quad (\text{E.1})$$

There are two residuals, one for the current solution, φ_i , and one for the corrected solution, $\tilde{\varphi}_i$.

$$r_i = b_i - \left(a_i^p \varphi_i + \sum_{nb} a_i^{nb} \varphi_{nb} \right) \quad (\text{E.2})$$

$$\tilde{r}_i = b_i - \left(a_i^p \tilde{\varphi}_i + \sum_{nb} a_i^{nb} \tilde{\varphi}_{nb} \right) \quad (\text{E.3})$$

Control volume i and some of its neighbours are designated as belonging to control volume I in a coarser grid. A corrected solution, $\tilde{\varphi}_i$ is sought for fine control volume i such that

the residuals (or flux errors) of i and all of the other control volumes in block I sum to zero.

$$\sum_{i \in I} \tilde{r}_i = 0 \quad (\text{E.4})$$

We define a correction, Φ_I , which is computed for block I .

$$\bar{\varphi}_i = \varphi_i + \Phi_I \quad (\text{E.5})$$

Some of the neighbouring points φ_{nb} of φ_i lie within coarse volume I , while others are found in neighbouring coarse volumes. The notation Φ_{nb^*} represents coarse volume values which contain the neighbour points of φ_i . If all neighbours of φ_i lie within coarse volume I , then nb^* and I are equivalent. Hence, the residual for the corrected solution is given by the following.

$$\begin{aligned} \tilde{r}_i &= b_i - \left[a_i^p (\varphi_i + \Phi_I) + \sum_{nb} a_i^{nb} (\varphi_{nb} + \Phi_{nb^*}) \right] \\ &= b_i - a_i^p \varphi_i - a_i^p \Phi_I - \sum_{nb} a_i^{nb} \varphi_{nb} - \sum_{nb} a_i^{nb} \Phi_{nb^*} \\ &= r_i - a_i^p \Phi_I - \sum_{nb} a_i^{nb} \Phi_{nb^*} \end{aligned} \quad (\text{E.6})$$

Summing the above equation over all fine volumes i in block I , the following is obtained.

$$\sum_{i \in I} \tilde{r}_i = \sum_{i \in I} r_i - \sum_{i \in I} a_i^p \Phi_I - \sum_{nb} a_i^{nb} \Phi_{nb^*} \quad (\text{E.7})$$

However, Equation (E.4) indicates the left-hand side of the above equation is equal to zero. Thus, the following is obtained.

$$\sum_{i \in I} a_i^p \Phi_I + \sum_{i \in I} \sum_{nb} a_i^{nb} \Phi_{nb^*} = \sum_{i \in I} r_i \quad (\text{E.8})$$

A change of variables is performed. A_I^{NB} is equal to the sum of all fine grid coefficients a_i^{nb} which multiply the same Φ_{nb^*} . Further, $B_I = \sum_{i \in I} r_i$. This represents the sum of the residuals in fine volume i . This change of variables permits us to sum over the ‘true’ neighbour points of I (i.e. Φ_{NB}) as opposed to the points I which contain neighbour points of φ_i (i.e. Φ_{nb^*}).

$$A_I^p \Phi_I + \sum_{NB} A_I^{NB} \Phi_{NB} = B_I \quad (\text{E.9})$$

Compare the above equation to Equation (E.1). The form is identical, which implies that residual errors in Equation (E.9) can themselves be raised to a higher frequency through grid coarsening. The recursive nature of this method requires a ‘stopping condition’ at which further grid coarsening is halted, and the cascade of finer grid values

Figure E.1: Multigrid ‘W-cycle’

corrected *via* Equation (E.5). The target number of multigrid levels is determined by the parameters `mgmin` and `mgmax`, which set the minimum and maximum number of control volumes concatenated together in each coarsening step. The lowest multigrid level is reached when a subsequent coarsening would yield less than `mgmin` control volumes. This level, therefore, is a function of the number of control volumes as well as the coefficients which are used to group the control volumes.

Note that application of Equation (E.9) represents a passing of information from a fine grid to a coarser one, while application of Equation (E.5) represents information flow in the opposite direction. Maintaining an effective transfer of error and corrector information between fine grids to coarser grids is the reason for TASCflow’s use of a ‘W-cycle’ approach to multigrid.

A ‘W-cycle’ consists of a series of steps down to the target coarseness level, followed by a single step back towards the fine grid. After the single step back, an additional ‘backtrack’ is made down to the coarse grid. Only after returning from the ‘backtrack’ is a step up to the finer grid permitted to occur. The process then repeats itself, with steps down to the target coarseness level followed by one step up, *etc.*. Graphically, this procedure traces a ‘W’ figure, as illustrated in Figure E.1.

The benefit of a ‘W-cycle’ is that a grid at a particular coarseness level is provided with two ‘installments’ of correction information from the lower, coarser grid prior to passing its correction information to the higher, finer grid. For example, grid coarseness level ‘3’ in Figure E.1 receives correction information from level ‘4’ twice prior to passing correction information to level ‘2’. Note that ‘2’, in turn, requires correction information from level ‘3’ twice prior to passing information back up to the original fine grid.

Appendix F

Table of Experimental Datasets

Table F.1: Table of Experimental Rod Bundle Datasets
Datasets

Reference	Rating	geometry				p/D ratio, γ_p	fluid		Reynolds range	Measurements				
		triangular	square	wall	gap only		air	water		secondary flows	Reynolds stress	thermal mixing	eddy viscosity	wall shear
Bartzis [24]	**	•				1.12		•	$9 \times 10^3 - 7 \times 10^4$		•			
Bishop [71]	*	•		•		1.2		•	?					
Carajilescov [18]	***	•				1.12		•	3×10^4		•			•
Castellana [33]	**		•			1.33		•	$9 \times 10^3 - 5 \times 10^5$			•		
Hetsroni [26]	**		•			1.25		•	$2 \times 10^4 - 4 \times 10^4$				•	
Hishida [6]	*	n/a ¹				n/a	•		4×10^4					

¹Hishida investigated a circular pipe

Table F.1: (continued)

Reference	Rating	geometry				p/D ratio, γ_p	fluid		Reynolds range	Measurements				
		triangular	square	wall	gap only		air	water		secondary flows	Reynolds stress	thermal mixing	eddy viscosity	wall shear
Krauss [4]	***			•		1.12	•		7×10^4		•		•	•
Krett [72]	*	•				?	•		$4 \times 10^4 - 2 \times 10^5$					
Meyer [5]	***	•				1.12	•		7×10^4		•		•	
Möller [73]	*	•		•		1.3	n/a ²		$3 \times 10^4 - 8 \times 10^4$					
Möller [48]	***			•		1.0 - 1.2	•		$2 \times 10^4 - 2 \times 10^5$		•			
Rapier [40]	**		•		•	1.2 - 1.6	•		5×10^4			•		
Rehme [19]	***			•		1.1 - 1.4	•		$9 \times 10^4 - 2 \times 10^5$		•		•	•
Rehme [14]	**	•		•		1.0 - 2.3		•	$8 \times 10^3 - 2 \times 10^5$					
Rehme [74]	*	•		•		1.1 - 1.4	•		$4 \times 10^3 - 8 \times 10^4$					
Rehme [16]	***			•		1.1 - 1.15	•		8×10^4		•			
Rehme [7]	***			•		1.1	•		9×10^4		•			•

²Möller's working fluid was sodium

Table F.1: (continued)

Reference	Rating	geometry				p/D ratio, γ_p	fluid		Reynolds range	Measurements				
		triangular	square	wall	gap only		air	water		secondary flows	Reynolds stress	thermal mixing	eddy viscosity	wall shear
Renksizbulut [15]	***		•	•		1.15		•	5×10^5		•			•
Rogers [39]	***	•				1.4	•		$9 \times 10^3 - 5 \times 10^4$			•		
Roidt [36]	**	•				1.25	•		7×10^4			•		
Rowe [75]	**		•	•		1.2 -		•	$5 \times 10^4 - 2 \times 10^5$		•			
Sadatomi [76]	-				•	n/a	•	•	n/a					
Sato [77]	-				•	n/a	•	•	n/a					
Seale [37]	****			•		1.1 - 1.83	•		$3 \times 10^4 - 3 \times 10^5$			•		
Seale [22]	***			•		1.2	•		2×10^5	•	•			
Skinner [78]	**	•		•		1.3	•		$2 \times 10^4 - 1 \times 10^5$			•		
Trupp [20]	***	•				1.2 - 1.5	•		$2 \times 10^3 - 8 \times 10^4$		•			•
Van Der Ros [35]	**				•	n/a		•	$5 \times 10^4 - 3 \times 10^5$			•		
Vonka [45]	***	•				1.3		•	$6 \times 10^4 - 2 \times 10^5$	•				

Table F.1: (continued)

Reference	Rating	geometry				p/D ratio, γ_p	fluid		Reynolds range	Measurements				
		triangular	square	wall	gap only		air	water		secondary flows	Reynolds stress	thermal mixing	eddy viscosity	wall shear
Wu [79]	***			•		1.15	•		6×10^4 - 7×10^4			•		•
Yang [80]	*		•			1.3		•	1×10^4 - 1×10^5					

Appendix G

Seale Experiment Mesh Generation Using TASCgrid

The computational domain required by the Seale experiment presented some mesh generation challenges. On the symmetry side of the domain cross section, the geometry is straight, while on the opposite side, the geometry is curved. Further, as wall functions are used to model the turbulent wall effects, correct placement of the internal nodes closest to the walls.

The topology of the mesh is based on a single fundamental ‘brick’ shape with eight nodes, twelve edges, and six surfaces. In order to create the geometry used in the Seale investigation, one side of the brick is bent into a semi-circle as illustrated in two dimensions in Figure G.1.

The side opposite the semi-circle is bent into three segments with a special vertex at each bend. The numbering of nodes from 1 to KD starts in the lower right-hand corner, moves along the base, up the left-hand side, and finishes along the top. In other words, from TASCgrid’s point-of-view, the bottom, left, and top curves are actually one line segment bent in two places. As a result, lines of constant K in the left-hand part of Figure G.1 become in the right-hand part ‘spokes’ emanating from the surface of the semi-circle.

This concept is crucial to understanding how nodes are defined and distributed around the mesh.

Figure G.1: Mesh Topology

G.1 Geometry Definition

G.1.1 Key Points

The geometry definition consists of two parts: the global parameter file and the geometry definition file (GDF).

The global parameter file defines the four key geometry control variables: pitch-to-diameter ratio, test section height, rod-to-rod pitch, and test section length. Only these four variables need be specified; all other geometry variables (*i.e.* rod radius, gap sizes, *etc*) are derived from these quantities. All variables are defined in meters. In all grid files, the term 'pin' is used to represent the rod.

The global parameter file is read into the geometry definition file (GDF). The GDF defines the points and curves which describe the flow domain.

The first part of the GDF defines the locations of key vertices based upon variables such as gap widths, section heights, *etc.*. The point definitions consist of a macro which is called twice, once for the 'east' (inlet) end of the section, and a second time for the 'west' (outlet) end. The locations of the inlet end nodes and vertices is provided in Figure G.2. The naming convention follows a set sequence based upon the 'compass' points indicated at the bottom of Figure G.2. Table G.1 provides a description of the naming convention.

The remainder of the GDF file defines the curves which connect the nodes and the

Figure G.2: Mesh Node Names

surfaces which are edged by the curves. As with the point definitions, macros are used for curve and surface definition.

A special macro called `define_inside_curves` creates six special 'inside' curves, three on the inlet, and three on the outlet. Named `inside_top_x`, `inside_middle_x`, and `inside_bottom_x` where x is e for the inlet and w for the outlet, these curves provide locations for defining the wall function control nodes. These special nodes are discussed further in the curve definition file (CDF) section.

G.1.2 global_parameters File

```
!      Global parameters for Seale Geometry

! If you change anything in this file, you will have to rerun:
! tascgridg --> tascgridc --> tascgrids --> tascgridi

! Pitch-to-diameter ratio
ed_ratio = 1.1

! Pitch between pins [m]
pin_pitch = 5.5e-2

! Pin diameter [m]
pin_diameter = pin_pitch / pd_ratio

! Pin radius [m]
```

Table G.1: Point Variable Naming Convention

format: point_(1)(2)(3)(4)		
position	letter	description
(1)	e	east ($-x$, inlet)
	w	west ($+x$, outlet)
(2)	n	north ($+y$)
	s	south ($-y$)
(3)	t	top ($+z$)
	b	bottom ($-z$)
(4)	i	inside
	o	outside

```

pin_radius = pin_diameter / 2.

! Gap between pins [m]
pin_half_gap = (pin_pitch - pin_diameter) / 2.

centre_x = 0.
centre_y = 0.
centre_z = 0.

! Length of test section [m]
section_length = 1.0

! Height of test section [m]
section_height = 6.86e-2

! Gap between pin and walls [m]
wall_gap = (section_height - pin_diameter) / 2.

```

G.1.3 GDF File

```

!      Geometry definition file for Seale Geometry
!
! There is nothing which requires editing here.

! If you wish to change the subchannel dimensions,
! edit the global_parameters file.

! If you wish to change the grid refinement,
! edit the cdf file.

VARIABLE DEFINITIONS

include global_parameters

```

```
define macro define_face_points
```

```
! Usage: define_face_points (w,e) (O, section_length)
```

```
    point_$inti (centre_x + $2, &
                  centre_y, &
                  centre_z + pin_radius)
```

```
    point_$into (centre_x + $2, &
                  centre_y, &
                  centre_z + pin_radius + wall_gap)
```

```
    point_$1st (centre_x + $2, &
                 centre_y - pin_radius - pin_half_gap, &
                 centre_z + pin_radius + wall_gap)
```

```
    point_$1s (centre_x + $2, &
                centre_y - pin_radius - pin_half_gap, &
                centre_z)
```

```
    point_$1sb (centre_x + $2, &
                 centre_y - pin_radius - pin_half_gap, &
                 centre_z - pin_radius - wall_gap)
```

```
    point_$1nbo (centre_x + $2, &
                  centre_y, &
                  centre_z - pin_radius - wall_gap)
```

```
    point_$1nbi (centre_x + $2, &
                  centre_y, &
                  centre_z - pin_radius)
```

```
    point_$1si (centre_x + $2, &
                 centre_y - pin_radius, &
                 centre_z)
```

```
    point_$1sti (centre_x + $2, &
                  centre_y - pin_radius * cos(pi/3.5), &
                  centre_z + pin_radius * sin(pi/3.5))
```

```
    point_$1sbi (centre_x + $2, &
                  centre_y - pin_radius * cos(pi/3.5), &
                  centre_z - pin_radius * sin(pi/3.5))
```

```
endmacro
```

```
define macro define_curves
```

```
! Usage: define_curves (w,e)
```

```
    curve pin_$1 radial R=pin_radius Axis = (-1,0,0)
    point_$1nbi; point_$1sbi; point_$1si; point_$1sti; point_$inti
```

```
    curve wall_gap_top_$1 linear
    point_$inti; point_$into
```

```

        curve wall_and_cl_$1 linear
        point_$1nto; point_$1st; point_$1s; point_$1sb; point_$1nbo

        curve wall_gap_bottom_$1 linear
        point_$1nbo; point_$1nbi

    endmacro

define macro define_inside_curve
! Usage:  define_inside_curve (w,e)
        curve inside_bottom_$1 linear
        point_$1sbi; point_$1sb

        curve inside_middle_$1 linear
        point_$1si; point_$1s

        curve inside_top_$1 linear
        point_$1sti; point_$1st
endmacro

define macro define_end_surfaces
! Usage:  define_end_surfaces (w,e)
        surface surf_$1 by curves bilinear
        pin_$1; wall_gap_top_$1; wall_and_cl_$1; wall_gap_bottom_$1

endmacro

define macro define_side_surfaces
! Usage:  define_side_surfaces
        surface surf_pin by curves linear
        pin_w; pin_e
        boundaries
        pin_b; pin_t

        surface surf_wall_gap_top by curves linear
        wall_gap_top_w; wall_gap_top_e
        boundaries
        pin_t; wall_t

        surface surf_wall_gap_bottom by curves linear
        wall_gap_bottom_w; wall_gap_bottom_e
        boundaries
        wall_b; pin_b

        surface surf_wall_and_cl by curves linear
        wall_and_cl_w; wall_and_cl_e
        boundaries
        wall_t; wall_b

endmacro

POINT

```

```

! Define points
define_face_points w 0.
define_face_points e section_length

! Define curves
define_curves w
define_curves e

! Add curves inside the surfaces (used for
! distributing first flow nodes)
define_inside_curve w
define_inside_curve e

! Define surfaces
define_end_surfaces w
define_end_surfaces e
define_side_surfaces

```

G.2 Curve Definition

G.2.1 Key Points

The curve definition file (CDF) assigns nodes along the curves defined by the GDF file. The nodes are assigned in three principle directions: axial, azimuthal, and radial. Figures G.1 and G.3 provide two-dimensional nodal coordinates for the J and K directions (the I direction is axial).

The first few lines of the CDF file specify the nodal density of the mesh. The ID parameter sets the number of axial nodes, JD sets the number of radial nodes¹

When selecting ID,JD, and KD, a number of points must be kept in mind.

1. Depending on the pitch-to-diameter ratio, the gap between the rods may be a very small space. Remember that the circumferential mesh lines (the number of which are specified by JD) become quite compressed in this area. As the circumferential mesh lines come closer together, the azimuthal mesh lines (the number of which are specified by KD) must also come closer together in the gap area.
2. ID must be a large enough number that the small control volumes in the gap region have an aspect ratio of 1:30 or smaller. Although the TASCflow User Manual

¹Note that radial nodes define the location of circumferential mesh lines, while azimuthal nodes define the location of radial mesh lines. Hence, the number of radial nodes equals the number of circumferential mesh lines, and the number of azimuthal nodes equals the number of radial mesh lines (see Figure G.3).

Figure G.3: Mesh Layout

suggests a control volume aspect ratio upper limit of 1:100, lower values produce better results.

3. The KD parameter should be a multiple of 6 plus 1. That is, KD values of $5 \times 6 + 1 = 31$, $9 \times 6 + 1 = 55$, *etc.* should be used. This is because the radial mesh lines (the number of which is controlled by KD) are divided by the CDF file into six groups. The first and sixth groups radiate from the rod surface to the bottom and top channel walls, respectively. The second through fourth groups radiate from the rod surface to the centreline symmetry line. This provides a higher density of radial mesh lines in the gap.

A number of variables are used to control the location of the internal nodes closest to the walls ($J = 2$ and $JD-1$). The correct placement of these nodes is important to the appropriate use of turbulent wall functions.

As seen in Table G.2 there are five control variables. These represent fractional distances from the rod surface to either the wall surface or the centreline depending on the application. In other words, `s1_gap_wall = 0.95` indicates that the node in question is to be placed 95% of the distance from the rod surface to the wall. The use of the `s1_` prefix arises from TASCgridc's node distribution syntax. When a node is being placed at a particular location, the variable `s1` is used to indicate a fractional distance as a function of the total segment length.

Table G.2: Wall Function Node Control Points

Variable	Description	Typical value ($\gamma_p = 1.1$)
sl_gap_wall	Near rod surface, gap between rod and wall	0.05
sl_wall_gap	Near wall surface, gap between rod and wall	0.95
sl_gap_cl	Near rod surface, gap between rod and centreline	0.25
sl_channel_pin	Near rod surface, gap between rod and intersection of centreline and wall	0.03
sl_channel_wall	Near wall surface, gap between rod and intersection of centreline and wall	0.95

Near the end of the definitions section of the CDF file are two variables called `r_ratio_1` and `r_ratio_2`. These control the density of lines of constant K (*i.e.*, radial nodes) in the rod-wall and rod-rod gaps, respectively. When `r_ratio_1` is increased, the lines of constant K (which are like spokes on a wheel) are ‘bunched’ closer together in the rod-wall gap both above and below the rod. Similarly, when `r_ratio_2` is increased, the lines of constant K are bunched closer together in the rod-rod gap.

G.2.2 CDF File

Grid Dimensions

! Number of nodes in axial direction (number of control volumes is one less)
ID=150

! Number of nodes between pin and wall (as well as number of nodes between
! pin and centreline)
JD=15

! Number of nodes around circumference of half-pin
! KD should be a multiple of 6 + 1 (*i.e.*, 25, 31, 37, etc.)
KD=55

! NOTE: if you change ID, JD, or KD, you will have to re-run the `define_regions`
! macro in TASCtool prior to using TASCbob3d.

! If you change anything in this file, you will have to rerun:
! `tascgridc --> tascgrids --> tascgridi`

Variable Definitions


```

! surf_w@st=(1,1)
! surf_wall_gap_top@st=(1,0)
! surf_wall_and_cl@st=(0,0)
point_wst      ( 1, 1, 5.*wallcvs + 1.)  ! Vertex # 7      wall_and_cl_w@p#2
! inside_top_w@p#2
point_ws       ( 1, 1, 3.*wallcvs + 1.)  ! Vertex # 8      wall_and_cl_w@p#3
! inside_middle_w@p#2
point_wsb      ( 1, 1, wallcvs + 1.)      ! Vertex # 9      wall_and_cl_w@p#4
! inside_bottom_w@p#2
point_wnbo     ( 1, 1, 1)                ! Vertex # 10     wall_and_cl_w@p#5
! wall_gap_bottom_w@p#1      wall_b@p#1
! surf_w@st=(0,1)
! surf_wall_gap_bottom@st=(0,0)
! surf_wall_and_cl@st=(1,0)
point_enbi     (ID,JD, 1)                ! Vertex # 11     pin_e@p#1
! wall_gap_bottom_e@p#2      pin_b@p#2
! surf_e@st=(0,0)
! surf_pin@st=(0,1)
! surf_wall_gap_bottom@st=(1,1)
point_esbi     (ID,JD, wallcvs + 1.)      ! Vertex # 12     pin_e@p#2
! inside_bottom_e@p#1
point_esi      (ID,JD, 3.*wallcvs + 1.)    ! Vertex # 13     pin_e@p#3
! inside_middle_e@p#1
point_esti     (ID,JD, 5.*wallcvs + 1.)    ! Vertex # 14     pin_e@p#4
! inside_top_e@p#1
point_enti     (ID,JD,KD)                ! Vertex # 15     pin_e@p#5
! wall_gap_top_e@p#1         pin_t@p#2
! surf_e@st=(1,0)
! surf_pin@st=(1,1)
! surf_wall_gap_top@st=(0,1)
point_ento     (ID, 1,KD)                ! Vertex # 16     wall_gap_top_e@p#2
! wall_and_cl_e@p#1         wall_t@p#2
! surf_e@st=(1,1)
! surf_wall_gap_top@st=(1,1)
! surf_wall_and_cl@st=(0,1)
point_est      (ID, 1, 5.*wallcvs + 1.)    ! Vertex # 17     wall_and_cl_e@p#2
! inside_top_e@p#2
point_es       (ID, 1, 3.*wallcvs + 1.)    ! Vertex # 18     wall_and_cl_e@p#3
! inside_middle_e@p#2
point_esb      (ID, 1, wallcvs + 1.)      ! Vertex # 19     wall_and_cl_e@p#4
! inside_bottom_e@p#2
point_enbo     (ID, 1, 1)                ! Vertex # 20     wall_and_cl_e@p#5
! wall_gap_bottom_e@p#1      wall_b@p#2
! surf_e@st=(0,1)
! surf_wall_gap_bottom@st=(0,1)
! surf_wall_and_cl@st=(1,1)

```

Node Distributions

Default=1

! start-vertex	end-vertex	expansion-factors	! curve label
point_wnbi	point_wsbi	100 @ r r_ratio_1	! pin_w
point_wsbi	point_wsi	100 @ r-r_ratio_1	! pin_w
point_wsi	point_wsti	100 @ r r_ratio_1	! pin_w
point_wsti	point_wnti	100 @ r-r_ratio_1	! pin_w

```

point_wnto      point_wst      100 @ r r_ratio_1 ! wall_and_cl_w
point_wst       point_ws       100 @ r-r_ratio_2 ! wall_and_cl_w
point_ws        point_wsb      100 @ r r_ratio_2 ! wall_and_cl_w
point_wsb       point_wnbo     100 @ r-r_ratio_1 ! wall_and_cl_w
point_enbi      point_esbi     100 @ r r_ratio_1 ! pin_e
point_esbi      point_esti     100 @ r-r_ratio_1 ! pin_e
point_esti      point_enti     100 @ r r_ratio_1 ! pin_e
point_enti      point_est      100 @ r r_ratio_1 ! wall_and_cl_e
point_ento      point_es       100 @ r-r_ratio_2 ! wall_and_cl_e
point_es        point_esb      100 @ r r_ratio_2 ! wall_and_cl_e
point_esb       point_enbo     100 @ r-r_ratio_1 ! wall_and_cl_e
point_wnbi      point_enbi     100 @ 1          ! pin_b
point_wnti      point_enti     100 @ 1          ! pin_t
point_wnto      point_ento     100 @ 1          ! wall_t
point_wnbo      point_enbo     100 @ 1          ! wall_b

point_wnti point_wnto 100 @ 1, sl = sl_gap_wall, n = 1,
    100 @ 1, sl = sl_wall_gap, n = JD - 3    ! wall_gap_top_w
point_enti point_ento 100 @ 1, sl = sl_gap_wall, n = 1,
    100 @ 1, sl = sl_wall_gap, n = JD - 3    ! wall_gap_top_e
point_wnbi point_wnbo 100 @ 1, sl = sl_gap_wall, n = 1,
    100 @ 1, sl = sl_wall_gap, n = JD - 3    ! wall_gap_bottom_w
point_enbi point_enbo 100 @ 1, sl = sl_gap_wall, n = 1,
    100 @ 1, sl = sl_wall_gap, n = JD - 3    ! wall_gap_bottom_e

point_wsti point_wst 100 @ 1, sl = sl_channel_pin, n = 1,
    100 @ 1, sl = sl_channel_wall, n = JD - 3    ! inside_top_w
point_esti point_est 100 @ 1, sl = sl_channel_pin, n = 1,
    100 @ 1, sl = sl_channel_wall, n = JD - 3    ! inside_top_e
point_wsi point_ws 100 @ 1, sl = sl_gap_cl, n = 1, 100 @ 1    ! inside_middle_w
point_e si point_es 100 @ 1, sl = sl_gap_cl, n = 1, 100 @ 1    ! inside_middle_e
point_wsbi point_wsb 100 @ 1, sl = sl_channel_pin, n = 1,
    100 @ 1, sl = sl_channel_wall, n = JD - 3    ! inside_bottom_w
point_esbi point_esb 100 @ 1, sl = sl_channel_pin, n = 1,
    100 @ 1, sl = sl_channel_wall, n = JD - 3    ! inside_bottom_e

```

G.3 Surface Definition

G.3.1 Key Points

The feature of the surface definition file (SDF) which sets it apart from the default template (SDT) file generated by TASCgridc is the inclusion of elliptic interpolation regions. These are made on the inlet `surf_e` and outlet `surf_w` surfaces. The wall function control nodes are not moved by the surface generation.

The syntax to process the surface definition file is as shown.

```
TASCgrids -s4 -nl1m
```

The `-s4 -nl1m` switches allocate a large block of real memory and 1×10^6 bytes of logical memory.

G.3.2 SDF File

```
Region surf_w elliptic
surface surf_w
(1,1,1) (1,JD,KD)
```

```
Region surf_e elliptic
surface surf_e
(ID,1,1) (ID,JD,KD)
```

```
Region surf_pin
```

```
Region surf_wall_gap_top
```

```
Region surf_wall_gap_bottom
```

```
Region surf_wall_and_cl
```

G.4 Internal Definition

G.4.1 Key Points

There are no particular key points associated with the internal definition file (IDF). The file specifies two points which are at opposite diagonal corners of the octant (here, ‘west-north-bottom-outside’ and ‘east-north-top-inside’) and a name for the octant internal region (‘subchannel’).

G.4.2 IDF File

```
! Internal definition file
```

```
region subchannel
point_wnbo, point_entl
```

Appendix H

Modifications to TASCflow in Support of Two-dimensional Thermal Solution

The TASCflow program allows customization of some of its subroutines. Two subroutines were modified to support the calculation of the Seale experiment temperature field: `propt.f` and `userpp.f`. The subroutine `propt.f` reads the turbulence parameters from an input file and calculates the effective thermal conductivity, while `userpp.f` post-processes the temperature field and determines the gap Stanton number and ratios of gap velocities to maximum velocities.

H.1 TASCtool Macro `write_cond`

A TASCtool macro called `write_cond` is used to write the turbulence parameters (TKE and EPSILON) from the three-dimensional flow solution to an output file to be read in by the two-dimensional thermal solution. The axial velocity, U , is included in order to allow calculation of the bulk temperatures.

```
write pro pro_fields="_u 0. 0. 0. 0. tke epsilon" [145,,] pro_name="cond" to pro.cond
```

The resulting `pro.cond` file is used by the two-dimensional temperature solution. The macro `write_cond` is stored in the `gci` file with all other macros.

H.2 Subroutine `propt.f` Modifications

The `propt.f` subroutine of TASCflow specifies the thermal properties of the fluid. Modification of this routine allows the inclusion of turbulent thermal conductivity to be used in

a two-dimensional solution devoid of its own turbulence field calculations. The effective thermal conductivity, Γ_{eff} , is calculated using the following.

$$\Gamma_{eff} = \Gamma + \frac{c_p}{Pr_t} \frac{\rho c_\mu k^2}{\varepsilon} \quad (H.1)$$

The structure of `propt.f` is as follows.

1. The local variables are declared. As the calculation of the turbulent conductivity field requires some fluid and turbulence parameters (*i.e.* ρ , Pr_t , c_μ , *etc.*), these are accessed from the array `CONST`.
2. If this is the first call to `propt.f` (as determined by the static variable `NOT1ST`), the `TKE` and `EPSILON` fields are read from the file `pro.cond`. As the turbulent conductivity field does not change from iteration to iteration, the entire thermal conductivity field is calculated immediately using the formula:

```
MYCOND(LOOPJ,LOOPK) = (RHOFLD * CMU *
& TKE * TKE / EPSILON) * CVFLD / PRT + CONDFL
```

3. On subsequent calls to `propt.f`, the value of the thermal conductivity at a particular location is obtained from the `MYCOND` array.

The contents of `propt.f` are as follows.

```
C=====
C
C      SUBROUTINE PROPT(CONDL,CPHEAT,CVHEAT,
&          U,V,W,P,T,PHI,NPHI,XYZ,
&          ILABEL,LABEL,I,J,K,ID,JD,KD)
C
CSCDT Calculates thermal properties of the fluid/solid.
C
CSCDB
C  PROPT is a user specified routine that calculates thermal
C  properties of the fluid/solid.
C
C  Input:
C
C      ILABEL = 0   fluid
C              > 0   MCF component index
C              < 0   solid CHT object with label given by 'LABEL'
C      LABEL : character string identifying equation solved
C      U,V,W : Cartesian velocity components
C      P      : static pressure
C      T      : static temperature
C      PHI    : additional scalars
C      NPHI   : number of additional scalars
C      XYZ    : Cartesian coordinates of grid nodes
```



```

C      I,J,K : topological grid coordinates
C      ID,JD,KD : topological grid dimensions
C
C      Output:
C
C      CONDL : local thermal conductivity
C      CPHEAT : specific heat at constant pressure
C      CVHEAT : specific heat at constant volume
C
C      Local:
C
C      MAXMCF : work space parameter for multi-component fluids
C      POFF : pressure offset (level shift)
C      TOFF : temperature offset (level shift)
C      CONDFL : fluid conductivity
C      CONDSL : solid conductivity
C      CPFLD : fluid specific heat at constant pressure
C      CVFLD : fluid specific heat at constant volume
C      CCSOL : solid specific heat
C      SUTHER : logical variable indicating whether or not to use
C              Sutherland's law
C
C      Common Blocks:
C
C      /CONTRL/ is declared so that information can be added as needed
C              for desired equation of state.
C
C      IONUM : integer, unit numbers in CONTRL common block.
C      IARR : integer, integer switches in CONTRL common block.
C      RARR : real, real constants in CONTRL common block.
C      CONST : real, property constants in CONTRL common block.
C      LARR : logical, logical switches in CONTRL common block.
C
C      /MULTIF/ contains information for multicomponent fluids.
C
C      DENSQ : real, component density.
C      ZMOLQ : real, component molecular weight.
C      CONDQ : real, component conductivity.
C      CPHTQ : real, component specific heat at constant pressure.
C      CVHTQ : real, component specific heat at constant volume.
C      LMCFQ : logical, multi-component fluid.
C      EQSTQ : logical, equation of state.
C      NMCF : integer, number of components.
C      NMCFNA : integer, maximum scalar which is a multi-component fluid.
C
C      NOTE: The true levels of pressure (P) and temperature (T) are
C            assumed to be
C             $P_{\text{true}} = P + \text{POFF}$ 
C             $T_{\text{true}} = T + \text{TOFF}$ 
C            where POFF and TOFF are level shifts in the actual dependent
C            values of P and T that are solved for.
CSCDE
C
C=====

```

```

C
C-----
C Subroutine Arguments
C-----
C
      INTEGER NPHI,I,J,K,ID,JD,KD,ILABEL
C
      REAL U(ID,JD,KD),V(ID,JD,KD),W(ID,JD,KD),P(ID,JD,KD),T(ID,JD,KD),
&      PHI(ID,JD,KD,*),XYZ(ID,JD,KD,3),CONDL,CPHEAT,CVHEAT
C
      CHARACTER*(*) LABEL
C
C-----
C Local Variables
C-----
C
      INTEGER MAXMCF
      PARAMETER (MAXMCF = 100)
C
      REAL CONDFL,CPFLD,CVFLD,CONDSL,CCSOL,POFF,TOFF
C
      LOGICAL SUTHER,ASCPRP

C RCKR Mod ---->

C      MYCOND:  My nodally dependent thermal conductivity
C               The 'ID' index is not required as the conductivity
C               is constant in the x direction.

C      NOT1ST:  Flags true if this is not the first call
C               to this routine

C      DUMMYx:  Five dummy variables used while reading in the
C               PRO.COND file.

C      xNODE:   Three integer variables which store the node
C               number for each line of the PRO.COND file.

C      LOOPx:   Two variables used to loop the J and K indices.

C      NODES:   Number of nodes in the pro.cond file

C      PRNAME:  Name of profile in pro.cond file

      INTEGER MAXJ, MAXK
      PARAMETER (MAXJ = 100)
      PARAMETER (MAXK = 100)

      REAL MYCOND(MAXJ, MAXK)
      LOGICAL NOT1ST
      REAL DUMMY1, DUMMY2, DUMMY3, DUMMY4, DUMMY5
      INTEGER INODE, JNODE, KNODE
      INTEGER LOOPJ, LOOPK
      INTEGER NODES

```

```

      CHARACTER*80 PRNAME
C <--- RCKR Mod
C
C-----
C Common Blocks
C-----
C
      COMMON/CONTRL/ IONUM(100),IARR(200),RARR(100),CONST(100),LARR(200)
      INTEGER IONUM,IARR
      REAL RARR,CONST
      LOGICAL LARR
C
      EQUIVALENCE (CONST(3),CONDFL),(CONST(11),CPFLD),(CONST(12),CVFLD),
&                (CONST(29),CONDSL),(CONST(30),CCSOL),
&                (CONST(13),POFF),(CONST(14),TOFF),(LARR(83),SUTHER),
&                (LARR(194),ASCPRP)
C
C RCKR Mod --->
C   RHOFLD: Density of fluid
C   PRT:    Turbulent prandtl number
C   CMU:    Turbulence constant (k-epsilon model)

      REAL RHOFLD, PRT, CMU

      EQUIVALENCE (CONST(1),RHOFLD),(CONST(4),PRT),(CONST(8),CMU)
C <--- RCKR Mod

      COMMON /MULTIF/ DENSQ(MAXMCF),ZMOLQ(MAXMCF),
&                  CONDQ(MAXMCF),CPHTQ(MAXMCF),CVHTQ(MAXMCF),
&                  LMCQ(MAXMCF),EQSTQ(MAXMCF),NMCQ,NMCFNA
      INTEGER NMCQ,NMCFNA
      REAL DENSQ,ZMOLQ,CONDQ,CPHTQ,CVHTQ
      LOGICAL LMCQ,EQSTQ
C
C-----
C Executable Statements
C-----
C
C----- SINGLE-COMPONENT FLUID
C
      IF (ILABEL.EQ.0) THEN
C
C-----
C----- USE SUTHERLAND'S LAW FOR THERMAL CONDUCTIVITY -----
C
      IF (SUTHER) THEN
        CONDL = 2.502E-3*(T(I,J,K)+TOFF)**1.5/(T(I,J,K)+TOFF+194.4)
      ELSE
C        CONDL = CONDFL
C RCKR Mod --->
C Determine if this is the first call to this routine
      IF (.NOT.NOT1ST) THEN

```

```

C      ----- READ PRO.COND FILE -----
C
C      The pro.cond file is generated from within TASCtool using
C      the 'write pro' command and the following syntax:
C
C      write pro pro_fields = "_u. 0. 0. 0. 0. tke epsilon" outlet to pro.cond
C
C      There is a check to make sure that the number of nodes required in this
C      run equal those available in the PRO.COND file.
      OPEN(FILE="pro.cond", UNIT=77, STATUS="old")

      READ(77,*) PRNAME
      READ(77,*) NODES, IB, JB, KB, IE, JE, KE

      IF(JE.GT.MAXJ.OR.KE.GT.MAXK) THEN
        PRINT *, "Error: pro.cond file has a grid which"
        PRINT *, "exceeds the maximum size available in the"
        PRINT *, "custom PROPT.F subroutine."
        PRINT *, "Maximum size: (",MAXJ,"x",MAXK,")"
        PRINT *, "Required size: (",JE,"x",KE,")"
        PRINT *, "Please increase MAXJ and/or MAXK in the"
        PRINT *, "routine PROPT.F accordingly."
        STOP
      ENDIF

C      IF(JE.NE.JD.OR.KE.NE.KD) THEN
C        PRINT *, "Error: pro.cond file has a grid which is"
C        PRINT *, "(",JE,"x",KE,") while grd file has grid"
C        PRINT *, "which is (",JD,"x",KD,")"
C        STOP
C      ENDIF

      DO LOOPK = KB, KE
        DO LOOPJ = JB,JE
          READ(77,*) INODE, JNODE, KNODE,
&          DUMMY1, DUMMY2, DUMMY3, DUMMY4, DUMMY5,
&          TKE, EPSILON

          MYCOND(LOOPJ,LOOPK) = (RHOFD * CMU *
&          TKE * TKE / EPSILON) * CVFLD / PRT + CONDFL

          END DO
        END DO

      CLOSE(UNIT=77)

      NOT1ST = .TRUE.
    ENDIF

    CONDL = MYCOND(J,K)

C <--- RCKR Mod
      ENDIF
C

```

```

C-----
      CPHEAT = CPFLD
      CVHEAT = CVFLD
C
C----- MULTI-COMPONENT FLUID COMPONENT
C
      ELSE IF (ILABEL.GT.0) THEN
C
      IF(ASCPRP) THEN
C          The unit of Cp and Cv is already converted in PRPCP
C          control parameter UNITS :
C          =1: SI (default)
C          =2: cgs/K
C          =3: lbm/in/s/R
C          =4: slug/ft/s/R
C
      CALL PRPCP(CPHEAT,CVHEAT,T,ILABEL,I,J,K,ID,JD,KD)
      ELSE
      CPHEAT = CPHTQ(ILABEL)
      CVHEAT = CVHTQ(ILABEL)
      ENDIF
C
      CONDL = CONDQ(ILABEL)
C
C----- USE SOLID DEFAULT THERMAL PROPERTIES
C
      ELSE
      CONDL = CONDSL
      CPHEAT = CCSOL
      CVHEAT = CCSOL
      ENDIF
C
      RETURN
      END

```

H.3 Subroutine userpp.f Modifications

The userpp.f subroutine provides user post-processing capability and is called after TASCflow has completed its run.

The quantities calculated by userpp.f include the following.

1. bulk velocity, UBULK;
2. areas of each control volume, AREACV;
3. area of the domain cross-section, AREAXS;

- The gap Stanton number is scaled to the top wall flux because q' along the top wall is not known in this subroutine.

```
C=====
C
SUBROUTINE USERPP (U,V,W,UNIP,P,T,TCOR,TKE,EPS,RHO,RHOIP,
& VISCT,PROP,XYZ,QVOL,CVOL,FEPC,PHI,NPHI,
& NBCF,IBCF,RBCF,NBLKF,NBNDIF,NBNDRF,
& NBCT,IBCT,RBCT,NBLKT,NBNDIT,NBNDRT,
& NBCS,IBCS,RBCS,NBLKS,NBNDIS,NBNDRS,
& NBCK,IBCK,RBCK,NBLKK,NBNDIK,NBNDRK,
& NBCE,IBCE,RBCE,NBLKE,NBNDIE,NBNBRE,
& NBKA,IBKA,NBLKA,NBKDIA,
& NBCQ,IBCQ,RBCQ,NBLKQ,NBLKQD,NBLKQM,
& NBNDIQ,NBNDRQ,
& WALVAL,NBNDRW,WRK,NWRK,IWRK,NIWRK,
& IPST,ITRM,IOUT,IBLOCK,IRSO,IWRFMT,
& N72,ID,JD,KD)
C
CSCDB USERPP is a user-supplied post-processing subroutine.
C
C The common block /CONTRL/ is declared here so that information
C can be added as needed for the desired equation of state.
C
C Input:
C
C U,V,W - velocity components in x,y and z directions
C P - pressure
C T,TCOR - temperature, corrected temperature (at walls, etc.)
C TKE,EPS - turbulent kinetic energy, dissipation rate
C RHO - density
C UNIP,RHOIP - velocity and density at integration points
C VISCT - turbulent viscosity
C PROP(I,J,K,IVISC) - laminar viscosity
C PROP(I,J,K,ICOND) - thermal conductivity
C PROP(I,J,K,ICPHT) - specific heat at constant pressure
C PROP(I,J,K,ICPVT) - specific heat at constant volume
C PROP(I,J,K,ISCALR + (N-1)) - N th scalar diffusion coefficient
C XYZ - x,y and z components of grid nodes
```

```

C   QVOL      - volume of each of the eight octants of each flux
C               element
C   CVOL      - volume of each complete control volume, including any
C               blockage and/or finite porosity effects.
C   FEPC      - porosity factor (fluid volume divided by
C               total volume)
C   PHI,NPHI  - additional scalars, number thereof
C   NBCF ... NBNDRW - arrays used to define boundary conditions
C   WRK,NWRK  - real workspace, size thereof
C   IWRK,NIWRK - integer workspace, size thereof
C   IPST,ITRM - output units for user post-processing,
C   IOUT,IRSO - terminal, standard output, RSO file
C   IBLOCK    - max block size for unformatted writes to RSO file
C   IWRFMT    - controls format of RSO file
C   N727      - number of elements in differencing scheme
C   ID,JD,KD  - grid dimensions
C   XYZ       - Cartesian coordinates of grid nodes
C
C   Local:
C
C       IFMT   - file format
C   NERR,IOERR - error flags
C       NAME   - file name
C
C   Common Blocks:
C
C   /CONTRL/ is declared so that information can be added as needed
C           for desired equation of state.
C
C       IONUM  : integer, unit numbers in CONTRL common block.
C       IARR   : integer, integer switches in CONTRL common block.
C       RARR   : real, real constants in CONTRL common block.
C       CONST  : real, property constants in CONTRL common block.
C       LARR   : logical, logical switches in CONTRL common block.
C
C   /FEGEOM/ contains shape function and surface normal
C           definitions within a finite element.
C
C       DNDL   : real, shape function derivatives w.r.t. local coords.
C       TRILIN : real, shape function values (tri-linear and linear-linear
C               interpolations both stored), for each of the 12 i.p.'s
C       QUADLN : real, shape function values (tri-linear and linear-linear
C               interpolations both stored), for each of the 8 octants.
C
C   /MAPS/ contains flux element topology map information.
C
C       INP    : integer, element local to global map for I index.
C       JNP    : integer, element local to global map for J index.
C       KNP    : integer, element local to global map for K index.
C       ILNB   : integer, I c.v. neighbor pointer relative to c.v. node.
C       JLNB   : integer, J c.v. neighbor pointer relative to c.v. node.
C       KLNB   : integer, K c.v. neighbor pointer relative to c.v. node.
C       NCMV   : integer, gives octant number in negative mass flow
C               direction, for each integration point location.

```

```

C      NCVF      : integer, gives octant number in positive mass flow
C                  direction, for each integration point location.
C      NPMAP     : integer, NPMAPB(ip_number, np_number) = np_num_active
C                  where ip_number is the element i.p. number (1-12),
C                  np_number is the node that a coefficient multiplies
C                  and np_num_active is the node number where the coeff.
C                  should actively be stored.
C      LPMAP     : integer, LPMAP(c.v._number, node_number) = nb_number
C                  where c.v._number is the local c.v. number (1-8) and
C                  node_number is the local node number that a given
C                  coefficient multiplies (1-8). The nb_number is the
C                  coefficient number for storage in a 27 point equation
C                  molecule (1-27).
C
C      /IPROP/ contains pointers into PROP array for fluid properties.
C
C      IVISC     : integer, pointer into PROP array for dynamic viscosity.
C      ICOND     : integer, pointer into PROP array for conductivity.
C      ICPHT     : integer, pointer into PROP array for specific heat, Cp.
C      ICVHT     : integer, pointer into PROP array for specific heat, Cv.
C      ISCALR    : integer, pointer into PROP array for Phi eqn diffusivity.
C
C      /PHINUM/ contains scalar transport equation information.
C
C      IARRQ     : integer, integer switches in PHINUM common block.
C      RARRQ     : real, real constants in PHINUM common block.
C      LARRQ     : logical, logical switches in PHINUM common block.
CSCDE
C
C=====
C
C-----
C Subroutine Variables
C-----
C
C      INTEGER NPHI,NBLKF,NBNDIF,NBLKT,NBNDIT,
C      &        NBNDRT,NBLKS,NBNDIS,NBNDRS,NBLKK,
C      &        NBNDIK,NBNDRK,NBLKE,NBNDIE,NBNDRF,NBNDRE,
C      &        NBLKA,NBNDIA,NBLKQD,NBLKQM,NBNDIQ,NBNDRQ,
C      &        NBNDRW,NWRK,NIWRK,IPST,ITRM,IOUT,IBLOCK,IRSO,IWRFMT,
C      &        N727,ID,JD,KD,
C      &        NBCF(NBLKF,4),IBCF(NBNDIF),NBCT(NBLKT,4),IBCT(NBNDIT),
C      &        NBKS(NBLKS,4),IBCS(NBNDIS),NBCK(NBLKK,4),IBCK(NBNDIK),
C      &        NBCE(NBLKE,4),IBCE(NBNDIE),NBKA(NBLKA,4),IBCA(NBNDIA),
C      &        NBLKQ(NBLKQD,*),NBCQ(NBLKQM),IBCQ(NBNDIQ),
C      &        IWRK(NIWRK)
C
C      REAL U(ID,JD,KD),V(ID,JD,KD),W(ID,JD,KD),UNIP(ID,JD,KD,12),
C      &      P(ID,JD,KD),T(ID,JD,KD),TKE(ID,JD,KD),EPS(ID,JD,KD),
C      &      RHO(ID,JD,KD),RHOIP(ID,JD,KD,12),VISCT(ID,JD,KD),
C      &      PROP(ID,JD,KD,*),
C      &      XYZ(ID,JD,KD,3),QVOL(ID,JD,KD,8),CVOL(ID,JD,KD),
C      &      FEPC(ID,JD,KD),WRK(NWRK),WALVAL(NBNDRW),TCOR(ID,JD,KD),
C      &      PHI(ID,JD,KD,*)

```



```

      REAL RBCF(NBNDRF),RBCT(NBNDRT),RBCS(NBNDRS),RBCK(NBNDRK),
&      RBCE(NBNDRE),RBCQ(NBNDRQ)
C
C-----
C Local Variables
C-----
C
C      INTEGER IFMT,NERR,IOERR
C
C      CHARACTER*80 NAME
C
C-----
C Common Blocks
C-----
C
C      COMMON/IPROP/ IVISC,ICOND,ICPHT,ICVHT,ISCALR
C      INTEGER IVISC,ICOND,ICPHT,ICVHT,ISCALR
C
C      COMMON/MAPS/ INP(8),JNP(8),KNP(8),ILNB(7),JLNB(7),KLNB(7),
&      NCVM(12),NCVP(12),NPMAP(12,8),LPMAP(8,8)
C      INTEGER INP,JNP,KNP,ILNB,JLNB,KLNB,NCVM,NCVP,NPMAP,LPMAP
C
C      COMMON/FEGEOM/DNDL(12,8,3,2),TRILIN(12,8,2),QUADLN(8,8,2)
C      REAL DNDL,TRILIN,QUADLN
C
C      COMMON/PHINUM/IARRQ(100,10),RARRQ(100,10),LARRQ(100,10)
C      INTEGER IARRQ
C      REAL RARRQ
C      LOGICAL LARRQ
C
C      COMMON/CONTRL/ IONUM(100),IARR(200),RARR(100),CONST(100),LARR(200)
C      INTEGER IONUM,IARR
C      REAL RARR,CONST
C      LOGICAL LARR
C
C RCKR Mod --->
C
C      AREACV: Area of a single control volume (y-z face)
C      To save memory, AREACV is a scalar and used
C      immediately within its own loop
C
C      AREAXS: Area of cross-section of domain (assumes that
C      y-z slices are flat)
C
C      INTEGER LOOPI, LOOPJ, LOOPK
C      INTEGER MAXI, MAXJ, MAXK
C      PARAMETER(MAXI=160,MAXJ=100,MAXK=100)
C
C      REAL AREACV
C      REAL AREAXS
C
C      REAL UHYB(MAXJ, MAXK)
C      REAL TBULKU, TBULKL, MDOT, MDOTL, MDOTU, MDOTCV

```

```

REAL DUMMY1, DUMMY2, DUMMY3, DUMMY4, DUMMY5, DUMMY6
INTEGER INODE, JNODE, KNODE
INTEGER LOOPJ, LOOPK
INTEGER NODES
CHARACTER*80 PRNAME

```

```

REAL DIST, GAPSIZ
REAL MAXY, MINY, YCOORD, WALLSZ
REAL STGAP, WPRIME

```

```

REAL MAXU, GAPU, WALLU, LOCALU, WALLUM
REAL MID_Z
LOGICAL FOUND

```

```

REAL RHOFD
EQUIVALENCE (CONST(1),RHOFD),(CONST(11),CPFLD)

```

```

C <--- RCKR Mod
C
C-----
C Executable Statements
C-----
C
C----- OTHER USER CUSTOMIZED SCALAR FIELDS TO PSAT, RSO AND/OR OUT FILE
C
C      CALL ASCOPN('PST',IPST,NAME,IFMT,' ',NERR,IOERR,1)
C      CALL RFOUTA(?,?, 'STUFF?',
C      &           IWRfmt,50,6,1,ID,1,JD,1,KD,1,1,ID,JD,KD,1,
C      &           IBLOCK,IRSO,ITRM,IOUT)
C      CALL OUT3D(?,?, 'STUFF?',
C      &           IWRK,IWRK(ID+1),1,1,1,IOUT,6,
C      &           1,ID,1,JD,1,KD,1,ID,1,JD,1,KD,XYZ)
C
C RCKR Mod --->
C      Check that maximum cv areas have not been exceeded.
C
      IF(ID.GT.MAXI.OR.JD.GT.MAXJ.OR.KD.GT.MAXK) THEN
        PRINT *, "Error: Maximum array sizes in user-defined"
        PRINT *, "routine USERPP.F have been exceeded."
        PRINT *, "Maximum array size is:"
        PRINT *, "(",MAXI,"x",MAXJ,"x",MAXK,")", however"
        PRINT *, "required array size is:"
        PRINT *, "(",ID,"x",JD,"x",KD,")". Please increase"
        PRINT *, "MAXI, MAXJ, and/or MAXK in USERPP.F."
        STOP
      END IF
C
C      ---- Read velocity data from PRO.COND file
      OPEN(FILE="pro.cond", UNIT=77, STATUS="old")
C
      READ(77,*) PRNAME
      READ(77,*) NODES, IB, JB, KB, IE, JE, KE

```

```

      IF(JE.GT.MAXJ.OR.KE.GT.MAXK) THEN
        PRINT *, "Error: pro.cond file has a grid which"
        PRINT *, "exceeds the maximum size available in the"
        PRINT *, "custom PROPT.F subroutine."
        PRINT *, "Maximum size: (",MAXJ,"x",MAXK,")"
        PRINT *, "Required size: (",JE,"x",KE,")"
        PRINT *, "Please increase MAXJ and/or MAXK in the"
        PRINT *, "routine PROPT.F accordingly."
        STOP
      ENDIF

C      IF(JE.NE.JD.OR.KE.NE.KD) THEN
C        PRINT *, "Error: pro.cond file has a grid which is"
C        PRINT *, "( ",JE,"x",KE,") while grd file has grid"
C        PRINT *, "which is ( ",JD,"x",KD,")"
C        STOP
C      ENDIF

      DO LOOPK = KB, KE
        DO LOOPJ = JB, JE
          READ(77,*) INODE, JNODE, KNODE,
&          UHYB(LOOPJ,LOOPK), DUMMY1, DUMMY2, DUMMY3,
&          DUMMY4, DUMMY5, DUMMY6

          END DO
        END DO

      CLOSE(UNIT=77)

      MDOTL = 0.
      MDOTU = 0.
      MDOT = 0.
      AREAXS = 0.
      TBULKL = 0.
      TBULKU = 0.

      LOOPI = (ID+1) / 2.

C      Cycle through nodes in cross-section

      DO LOOPJ = 1, JD
        DO LOOPK = 1, KD

C          Area of control volume
          AREACV = CVOL(LOOPI, LOOPJ, LOOPK) /
&          (0.5 * ( XYZ(LOOPI+1,LOOPJ,LOOPK,1)-
&          XYZ(LOOPI-1,LOOPJ,LOOPK,1)))

C          Mass flow through control volume
          MDOTCV = AREACV * RHOFLD * UHYB(LOOPJ,LOOPK)

```

```

C      Bulk temperature
C      -----
C      IF(LOOPK.LT.(KD+1)/2.) THEN
C          This is the lower half of the domain
C          TBULKL = TBULKL + MDOTCV * T(LOOPI,LOOPJ,LOOPK)
C          MDOTL = MDOTL + MDOTCV
C      ELSE IF(LOOPK.GT.(KD+1)/2.) THEN
C          This is the upper half of the domain
C          TBULKU = TBULKU + MDOTCV * T(LOOPI,LOOPJ,LOOPK)
C          MDOTU = MDOTU + MDOTCV
C      ELSE
C          This is the line right in the middle...
C          TBULKL = TBULKL + MDOTCV * T(LOOPI,LOOPJ,LOOPK) / 2.
C          MDOTL = MDOTL + MDOTCV / 2.
C          TBULKU = TBULKU + MDOTCV * T(LOOPI,LOOPJ,LOOPK) / 2.
C          MDOTU = MDOTU + MDOTCV / 2.
C      END IF

C      Cross sectional area
C      AREAXS = AREAXS + AREACV

C      Total cross-sectional flow (including middle)
C      MDOT = MDOT + MDOTCV

      END DO

      END DO

C      Find gap size by looking for smallest distance
C      between two nodes on the same KD line
C      GAPSIZ = 1.E10
C      DO LOOPK = 1, KD
C          DIST = SQRT((XYZ(1,1,LOOPK,2)-XYZ(1,JD,LOOPK,2))**2 +
C          &          (XYZ(1,1,LOOPK,3)-XYZ(1,JD,LOOPK,3))**2)

C          IF(DIST.LT.GAPSIZ) THEN
C              GAPSIZ = DIST
C          END IF

C      END DO

C      Determine width of top wall -- find the minimum and
C      maximum Y values in the system. This assumes the
C      subchannel is perpendicular to the Y/Z plane and the
C      face is aligned to the Y/Z axis (i.e., not rotated
C      around the x axis)
C      MAXY = -1.E10
C      MINY = 1.E10

C      DO LOOPK = 1, KD
C          YCOORD = XYZ(1,1,LOOPK,2)
C          IF(YCOORD.GT.MAXY) THEN
C              MAXY = YCOORD
C          END IF

```

```

      IF(YCOORD.LT.MINY) THEN
        MINY = YCOORD
      ENDIF
    END DO
    WALLSZ = MAXY - MINY

    TBULKL = TBULKL / MDOTL
    TBULKU = TBULKU / MDOTU
    UBULK = MDOT / (RHOFD * AREAXS)

    PRINT *, 'X-sec Area: ', AREAXS, ' [m^2]'
    PRINT *, 'Upper T_bulk: ', TBULKU, ' [K]'
    PRINT *, 'Lower T_bulk: ', TBULKL, ' [K]'
    PRINT *, 'M_dot: ', MDOT, ' [kg/s]'
    PRINT *, 'U_av: ', UBULK, ' [m/s]'
    PRINT *, 'Gap width: ', GAPSIZ, ' [m]'
    PRINT *, 'Top wall width: ', WALLSZ, ' [m]'

C    Calculate the gap Stanton number -- the
C    heat flux from the top wall is in the boundary
C    condition file and therefore unavailable to this
C    subroutine. Hence, calculate the Stanton number
C    in terms of the heat flux from the top wall.
    STGAP = WALLSZ / (GAPSIZ * (TBULKU - TBULKL) *
&      RHOFD * UBULK * CPFLD)

C    Calculate w' (again, in terms of the heat flux
C    from the top wall)
    WPRIME = STGAP * RHOFD * GAPSIZ * UBULK

    PRINT *, 'St_gap / Q_wall_flux: ', STGAP, ' [m^2/W]'
    PRINT *, 'w_prime / Q_wall_flux: ', WPRIME,
&      ' [kg m / s W]'

C    Find the maximum axial velocity
    MAXU = -1.E10
    DO LOOPJ = 1,JD
      DO LOOPK = 1, KD
        LOCALU = UHYB(LOOPJ,LOOPK)
        IF(LOCALU.GT.MAXU) THEN
          MAXU=LOCALU
        END IF
      END DO
    END DO

C    Get the velocity at the node(s) closest to
C    the centre of the pin-pin gap
    FOUND = .FALSE.
    MID_Z = (XYZ(1,1,1,3) + XYZ(1,1,KD,3))/2.
    LOOPK = 1.
    DO WHILE(.NOT.FOUND.AND.LOOPK.LE.KD)
      IF(XYZ(1,1,LOOPK,3) .GT. MID_Z) THEN
        FOUND = .TRUE.

```

```

        ELSE
            LOOPK = LOOPK + 1
        END IF
    END DO

C    At this point, LOOPK is pointing at the
C    first node with a z-coord greater than
C    the midplane.
    GAPU = UHYB(1,LOOPK-1) +
&      (UHYB(1,LOOPK) - UHYB(1,LOOPK-1)) *
&      (MID_Z - XYZ(1,1,LOOPK-1,3)) /
&      (XYZ(1,1,LOOPK,3)-XYZ(1,1,LOOPK-1,3))

C    Look for the maximum along a line from the pin to the wall
    WALLU = -1.E10
    DO LOOPJ = 1, JD
        LOCALU = UHYB(LOOPJ, KD)
        IF(LOCALU.GT.WALLU) THEN
            WALLU = LOCALU
        END IF
    END DO

C    Now look for the value at the midpoint between the pin
C    and the wall
    FOUND = .FALSE.
    MID_Z = (XYZ(1,1,1,3) + XYZ(1,JD,1,3))/2.
    LOOPJ = 1.
    DO WHILE(.NOT.FOUND.AND.LOOPJ.LE.JD)
        IF(XYZ(1,LOOPJ,1,3) .GT. MID_Z) THEN
            FOUND = .TRUE.
        ELSE
            LOOPJ = LOOPJ + 1
        END IF
    END DO

C    At this point, LOOPJ is pointing at the
C    first node with a z-coord greater than
C    the midpoint.
    WALLUM = UHYB(LOOPJ-1,1) +
&      (UHYB(LOOPJ,1) - UHYB(LOOPJ-1,1)) *
&      (MID_Z - XYZ(1,LOOPJ-1,1,3)) /
&      (XYZ(1,LOOPJ,1,3)-XYZ(1,LOOPJ-1,1,3))

    PRINT *, 'Maximum U: ', MAXU, ' [m/s]'
    PRINT *, 'Gap U: ', GAPU, ' [m/s]'
    PRINT *, 'Wall U: ', WALLU, ' [m/s]'
    PRINT *, 'Wall mid U: ', WALLUM, ' [m/s]'
    PRINT *, 'U_gap / U_max: ', GAPU / MAXU
    PRINT *, 'U_wall / U_max: ', WALLU / MAXU
    PRINT *, 'U_wall_mid / u_max: ', WALLUM / MAXU

C <--- RCKR Mod
    RETURN
END

```