COBRA-IV: The Model and the Method

by
C. W. Stewart, C. L. Wheeler,
R. J. Cena, C. A. McMonagle
J. M. Cuta, D. S. Trent

July 1977

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CONTENTS

LIST OF FIGURES	v
LIST OF TABLES	viii
1.0 INTRODUCTION	1
2.0 GOVERNING EQUATIONS	9
2.1 MIXTURE BALANCE LAWS	9
2.2 SUBCHANNEL EQUATIONS	15
2.2.1 Mass Balance	21
2.2.2 Energy Balance	22
2.2.3 Axial Momentum Balance	25
2.2.4 Lateral Momentum Balance	28
3.0 NUMERICAL SOLUTION	35
3.1 IMPLICIT SOLUTION	38
3.1.1 Difference Equations	41
3.1.2 Implicit Energy Equation	45
3.1.3 Momentum Equations	47
3.1.4 Solution Procedure	49
3.2 EXPLICIT METHOD	54
3.2.1 Difference Equations	57
3.2.2 The ACE Method	63
3.3 NUMERICAL PERFORMANCE	71
3.3.1 Transient Stability	72
3.3.2 Convergence	76
4.0 CONDUCTIVE HEAT TRANSFER	81
4.1 FUEL MODEL	81
4.1.1 Fuel Interior	82
4.1.2 Fuel-Clad Interface	86
4.1.3 Cladding	86
4.1.4 Solution Procedure	87
4.2 WALL MODEL	88
5.0 CONSTITUTIVE RELATIONS	93
5.1 FLUID STATE RELATION	94

5.1.1	Subcooled and Saturated Liquid Properties.	95
5.1.2	Two-Phase Properties	97.
5.1.3	Superheated Steam Properties.	99
5.2	HEAT TRANSFER CORRELATIONS.	101
5.2.1	Single Phase Flow	103
5.2.2	Two-Phase Flow	104
5.2.3	Critical Heat Flux Correlations.	105
5.3	FRICITION FACTOR AND LOSS COEFFICIENTS	108
5.3.1	Single-Phase Flow	109
5.3.2	Two-Phase Flow	110
5.4	TURBULENT MIXING	111
6.0	APPLICATIONS	115
6.1	COMPARISONS WITH ANALYTIC SOLUTIONS	116
6.1.1	Single-Limb Manometer	116
6.1.2	U-Table Manometer	118
6.1.3	Flow Decay Transient	118
6.2	DATA COMPARISONS	121
6.2.1	General Electric Nine-Rod Bundle Experiment.	122
6.2.2	Combustion Engineering Inlet Jetting Tests	124
6.2.3	Westinghouse Flow Blockage Tests	125
6.2.4	PNL Flow Blockage Experiments	127
6.2.5	Wire Wrap Application	133
6.2.6	Example of Application of COBRA to DNB Analysis	134
6.2.7	Semiscale Core Blowdown Calculations	136
6.2.8	Turbulent Plane Jet.	139
6.3	ILLUSTRATIONAL COMPUTATIONS	144
6.3.1	Isothermal Reflood Oscillation	144
6.3.2	Heated Reflood Oscillation	147
6.3.3	PWR Blowdown Calculations.	153
	REFERENCES	161
	APPENDIX - CONNECTION MATRIX EXAMPLES	A-1

FIGURES

2-1	Relation of Subchannel Control Volume to Reactor Core	16
2-2	Lateral Heat Conduction Problem	17
2-3	Subchannel Control Volume	20
2-4	Rod and Wall Surface Heat Transfer Geometry	23
2-5	Lateral Fluid Heat Conduction Geometry	24
2-6	Control Volume for Lateral Momentum	28
2-7	Gap Reference Angles	31
3-1	Placement of Variables for Implicit Solution	42
3-2	Implicit Solution Sequence	51
3-3	Placement of Primary Variables on a Computational Cell	58
3-4	Explicit Solution Sequence	68
4-1	Fuel Rod Noding Using Second Order Orthogonal Collocation	84
4-2	Fuel Conduction Matrix Elements	89
4-3	Conducting Wall Model Layout	90
5-1	Input Change for Zero Circumferential Conduction	103
5-2	Region of Application of Heat Transfer Correlations	105
6-1	Single-Limb Manometer Model	117
6-2	Undamped Single-Limb Manometer Results	117
6-3	U-Tube Manometer Model	119
6-4	Undamped U-Tube Manometer Results	119
6-5	Flow Decay Transient Quality Versus Time	120
6-6	Flow Decay Transient Mass Flux Versus Time	120
6-7	Comparison of Measured Versus Calculated Subchannel Exit Mass Velocities for the Single-Phase Isothermal Data	123
6-8	Comparison of Measured Versus Calculated Subchannel Exit Mass Velocities for the Two-Phase Data	123
6-9	Geometry of 15 x 15 Square Array Test Section	124

6-10	Subchannel Layout for CE Inlet Jetting Test	125
6-11	Inlet Jetting Test, Centerline Data	126
6-12	Inlet Jetting Test, Tangent Data	126
6-13	Data for Inlet Flow Distribution of 67 Percent/33 Percent	128
6-14	Data for Inlet Flow Distribution of 100 Percent/0 Percent	128
6-15	Axial Velocity Profiles for Westinghouse Flow Blockage Data	129
6-16	COBRA Geometry Model	131
6-17	COBRA Velocity Predictions in Subchannel #1 with a 70 Percent Blockage	131
6-18	Ninety Percent Blockage Velocity Profile	132
6-19	Velocity Profile for a 90 Percent Blockage Adjacent to a Spacer	132
6-20	COBRA Input for ORNL-FFM-2A Test Assembly	133
6-21	Comparison of Calculated and Measured Normalized Exit Temperatures in the Univormly Heated FFM-2A Test Assembly	134
6-22	Distribution of the MDNBR Values Calculated Using the B&W-2 DNB Correlation	137
6-23	Distribution of MDNBR Values Calculated Using the W-3S Correlation	137
6-24	Semiscale Core	138
6-25	Subchannel Model of the Semiscale Core	138
6-26	Comparison of Experimental and Calculated Core Inlet Density	140
6-27	Comparison of Experimental and Calculated Inlet Mass Flow Rate	140
6-28	Calculated Exit Mass Flow Rate	141
6-29	Turbulent Plane Jet Centerline Velocity Decay	143
6-30	Velocity Vector Field for Turbulent Plane Jet	143
6-31	PWR Core Model Showing Nonuniform Core Liquid Level	145
6-32	Water Level Oscillations with Uniform Initial Core Level	146
6-33	Water Level Oscillations with Nonuniform Initial Core Level	146

6-34	Liquid Level and Velocity, Uniform Power	148
6-35	Heat Transfer, Uniform Power	149
6-36	Axial Temperature Profile, Uniform Power	150
6-37	Transient Core Temperature Contours	152
6-38	Model of PWR Geometry for COBRA Calculations	154
6-39	Calculated Inlet Mass Velocities for Channels 1 and 6	155
6-40	Calculated Exit Mass Velocities for Channels 1 and 6	156
6-41	Calculated Flow Field in the PWR Core During the Blowdown Transient	157
6-42	Normalized Velocity Flow Field for PWR Core With and Without an Arbitrary Flow Blockage	160

TABLES

1-1	COBRA Development Chronology	3
2-1	Comparison of Classical and Subchannel Momentum Transport	34
3-1	Definition of Variables	37
3-2	Computation of Averages and Donor Cell Products	62
3-3	Summary of Explicit Time Step Restrictions	72
3-4	Equivalent Convergence Criteria	78
5-1	Typical Water Property Table	96
5-2	Typical Superheated Steam Property Table	100
5-3	Heat Transfer and Critical Heat Flux Correlations	106
6-1	Summary of COBRA Calculations	115
6-2	Classification of COBRA-IV Simulations for Data Comparison	121

COBRA-IV: THE MODEL AND THE METHOD

1.0 INTRODUCTION

The objective of this report is to present the mathematical basis of the COBRA-IV computer program (Wheeler et al., 1976) being developed by Battelle, Pacific Northwest Laboratory. The COBRA-IV code is an extended version of the COBRA-IIIC subchannel analysis code that computes the flow and enthalpy distributions in nuclear fuel rod bundles and cores for both steady state and transient conditions (Rowe, 1973).

Development of the COBRA computer code (from Coolant Boiling in Rod Arrays) through the COBRA-IIIC version was sponsored by the Atomic Energy Commission (AEC). Since the reorganization of the AEC, COBRA-IV has been under the sponsorship of both the Energy Research and Development Administration (ERDA) and the Nuclear Regulatory Commission (NRC). The ERDA sponsorship has been directed toward the Liquid Metal Fast Breeder Reactor (LMFBR), while the NRC has been concerned with improved computational and two-phase modeling for application to water reactor safety.

Over the past few years, COBRA has become widely accepted by the nuclear industry as a tool to help predict the thermal performance of nuclear fuel elements. It has been extensively used in the design and safety analysis of liquid metal, gas and water cooled reactor cores. It is a very powerful tool because it can be applied to the most complicated fuel configuration with relative ease.

COBRA utilizes the basic concept of subchannel analysis in which the flow area of a nuclear fuel rod bundle is divided into subchannels whose boundaries are defined by the adjacent fuel rod surfaces. The subchannels are divided axially into discrete control volumes for which the equations of continuity, energy, and momentum are written. Volume or surface averages define the dependent variables of mass flow rate, pressure, enthalpy and density.

Several methods have been employed to solve these subchannel conservation equations since the first version of COBRA was issued in 1967. Because each new solution procedure extended COBRA's range of application by building on the strengths of the previous version, it is convenient to trace the development of COBRA chronologically to gain a clear understanding of its present capabilities. There have been five stages in the development of COBRA since 1967: COBRA I, II, III, III-C and IV-I. The various features of each are summarized in Table 1-1. The following discussion explains the motivation for some of the major modifications.

The COBRA-I development was originally sponsored under a cooperative U.S. - Canadian program for the development of heavy water moderated reactors. It used a very simple pressure-resistance model for diversion of crossflows; the governing equations were solved with a forward marching technique restricting the code to positive axial flow and small crossflows in the steady state. A stability condition in transverse flow loops also governed the choice of axial node length and the lateral resistance coefficient.

This rather limited flow solution was retained in COBRA-II but the flexibility of the code was improved by adding correlations for two-phase turbulent mixing and subcooled voids, as well as a model for lateral heat conduction. Provision was also made for axial variation of subchannel gap and area.

TABLE 1-1. COBRA Development Chronology

<u>Capability or Model</u>	COBRA Version (Publication and Date)				
	I	II	III	IIIC	IV-1
	BNWL- 371 3/67	BNWL- 1229 2/70	BNWL-B- 82 7/71	BNWL- 1695 3/73	BNWL- 1962 5/76
Flow Solution - Steady State					
Forward March	x	x			
Inlet Flow/Exit Pressure					
Boundary Conditions			x	x	x
Pressure Drop					
Boundary Conditions					x
Flow Solution - Transient					
Full Implicit				x	x
Explicit Arbitrary Flow Field					
and Boundary Conditions					x
Single Phase Flow					
Nonuniform Channel Friction		x	x	x	x
Hot Wall Friction Correction				x	x
Laminar Friction Correction					x
Two-Phase Flow					
1-D Slip Flow	x	x	x	x	x
Subcooled Voids		x	x	x	x
Turbulent Mixing					
Single Phase	x	x	x	x	x
Two-Phase Models		x	x	x	x
Crossflow Model					
Pressure-Resistance Only	x	x	x		
Transient Momentum Equation				x	x
Forced Diversion				x	x
Lateral Momentum Flux					x
Equation of State					
Reference Pressure	x	x	x	x	x
Superheated Steam Properties					x
Geometry					
Variable Gap and Area		x	x	x	x
Grid Spacers		x	x	x	x
Blocked Crossflow (Transient)					x
Wire Wrap Spacer				x	x
Fluid Energy Solution					
Spatially Explicit	x	x	x	x	
Spatially Implicit					x
Heat Conduction - Fuel Rods					
Specified Axial and Radial					
Heat Flux	x	x	x	x	x
CHF Correlations				x	x
Transient Fuel Rod Model					
Finite Difference				x	
Orthogonal Collocation					x
Axial Conduction					x
Temperature-Dependent					
Conductivity					x
Axial Fuel Zones					x
Boiling Curve Package					x
Heat Conduction - Fluid					
Radial Conduction		x	x	x	x
Axial Conduction					x

Since much of the safety analysis for licensing and safe operation of nuclear reactors is related to the transient interaction of the fuel and coolant, the main objective after the release of COBRA-II was to develop transient subchannel analysis capability. Plans also called for a more complete transverse momentum equation, a wire wrap spacer model, a transient fuel heat conduction model, the elimination of the positive flow restriction and finally, pressure drop boundary condition capability.

The transient analysis capability was first made available in COBRA-III, which was released in the interim while development work continued on the remaining items. The numerical scheme adopted to solve the transient equations performed an iterative boundary value solution based on inlet flow, crossflow, and enthalpy and exit pressure with no numerical stability limitation on space or time step size. An important improvement over the original marching solution was the ability to calculate flow redistributions upstream of local disturbances.

The COBRA-IIIC version provided a significant improvement in the physical modeling. In addition to the transient capability of COBRA-III, the lateral momentum equation was improved by including both the temporal and spatial acceleration with the ability to consider forced flow diversion from wire wraps or diverter vanes. An implicit transient fuel conduction model was implemented to correctly model the thermal response of the fuel rods.

This coupled fuel-coolant transient model has been quite successfully applied to a wide variety of design and

safety analysis problems, including liquid metal and gas cooled systems. However, there are many areas where the inability to consider flow reversal and recirculation and the lack of a pressure boundary condition is very inconvenient. These include the analysis of postulated loss of coolant accidents and natural circulation in particular. The achievement of these capabilities was the major emphasis in the COBRA-IV development effort.

To provide these capabilities, a complementary independent solution scheme was developed for COBRA-IV since it proved impractical to modify the fully implicit COBRA-IIIC solution. After much experimentation, a temporally explicit transient pressure-velocity method was selected which imposed no restriction on flow direction and could accept either flow or pressure boundary conditions. It was necessary to modify this new method to compute the convective transport of internal energy implicitly to consider the propagation of sharp density gradients. This capability is required in the analysis of the reflood stage in loss of coolant accidents. The resulting numerical model, called the ACE method (for Advanced Continuous-fluid, Eulerian) is discussed in detail in Section 3.2 (Stewart and Rowe, 1976). The fully implicit COBRA-IIIC solution has been retained to provide an efficient steady-state calculation.

In addition to the new explicit transient option, COBRA-IV capabilities have been significantly extended by improvements made to the COBRA-IIIC fluid energy equation and to the transient fuel conduction model. The fluid energy equation used from COBRA-I through IIIC was

spatially explicit. That is, the fluid enthalpy at the current axial position was calculated using only information from the preceding axial position. While this allowed the enthalpy to be updated in a noniterative straightforward manner, it could not propagate an energy disturbance laterally across more than one channel per axial step. This was a source of computational instability at low flow rates in previous versions of COBRA. This problem has been eliminated in COBRA-IV by making the energy equation spatially implicit. All enthalpies at the same axial level are now calculated simultaneously by means of an iterative procedure. The details of this modification are discussed in Section 3.1.

The fuel rod conduction model has been made more efficient through the use of an orthogonal collocation method for radial heat conduction. Other new fuel model capabilities include options for considering axial conduction, temperature-dependent thermal conductivity, axial fuel zones with different fuel and clad materials and heat conducting walls between subchannels. These developments are described in Section 4.

The last column of Table 1-1 summarizes the current capabilities of COBRA-IV which have been introduced in the preceding paragraphs. The balance of this report will describe the mathematical bases for these capabilities in detail beginning with a derivation of the governing equations in Section 2. Section 3 is devoted to the numerical solution of these governing equations by the new explicit method (ACE) and by the improved implicit method from COBRA-IIIC. The improved fuel conduction model used by both the above flow field solutions is derived in Section 4.

The various constitutive relations used are outlined in Section 5. Section 6 presents a wide variety of COBRA-IV applications to both verify the code's performance and demonstrate many of its expanded capabilities.

These illustrations will show that COBRA-IV is fully two-dimensional and may now be extended to many situations far removed from subchannel geometry. The continuing development effort will broaden the code's applicability even further. Development goals include the capability to consider relative motion and thermal nonequilibrium between phases in two-phase flow and an expanded equation of state for treating compressible flows.

This document is intended to provide a base for reporting the results of succeeding development efforts. It is hoped that it will also complement the COBRA-IV user's manual in providing a clearer understanding of the capabilities and limitations of the code.

2.0 GOVERNING EQUATIONS

In this section, the general transient balance laws for mass, energy and linear momentum for a single component two-phase mixture are considered. The governing equations for subchannel geometry will be derived from integral balances on an arbitrary fixed (Eulerian) volume after Owczarek (1964). The two finite difference solution procedures used in COBRA-IV for the resulting set of equations are described in Section 3.

It is assumed that the mixture variables are sufficiently space-time averaged to provide continuous derivatives inside the fixed volume and over its surface. This permits smoothing of the chaotic nature of two-phase flow so that its essential nature can be considered. Averaging obviously removes detail from the balance equations, and when a computational grid and its associated time step limitations are imposed on a two-phase flow field through numerical techniques, resolution is further limited to the order of the space and time step [$O(\Delta x)$ and $O(\Delta t)$]. The physical, mathematical and numerical aspects of the modeling process cannot be studied separately.

2.1 MIXTURE BALANCE LAWS

The integral balances are formed on an Eulerian control volume, V , which is bounded by a fixed surface, A . This may consist of both a solid boundary, such as a fuel rod or structural wall, and a fluid boundary, but all fuel or other solid material is outside V . The energy balance

material thus excluded from V forms the fuel thermal model described in Section 4. The fluid in V is assumed to be a single component, two-phase mixture of liquid and vapor in thermodynamic equilibrium.

The local composition of the mixture is described by the space-time averaged vapor volume fraction, α . Any mixture variable, Q , can be expressed as the volume weighted sum of the individual phase variables, Q_v and Q_ℓ , as

$$Q = \alpha Q_v + (1-\alpha) Q_\ell \quad (2.1)$$

The integral balance for the arbitrary mixture property, Q , accounts for the change of the total amount of Q in V , the rate at which Q moves across the surface of V and the sum of all sources and sinks of Q inside V . If Q is defined in units/unit volume, the integral balance is written as

$$\frac{\partial}{\partial t} \int_V Q dV + \int_A Q (\vec{u} \cdot \vec{n}) dA = \int_V S dV \quad (2.2)$$

where $\vec{u}$ is the fluid velocity, $\vec{n}$ is the unit outward normal vector and S represents the net volumetric source of Q in V .

This derivation is concerned with the transport of mass, energy and momentum of the mixture as expressed by the variables

$$\begin{aligned} \rho &\equiv \alpha \rho_v + (1-\alpha) \rho_\ell \\ \rho &\equiv \alpha \rho_v e_v + (1-\alpha) \rho_\ell e_\ell \\ \rho \vec{u} &\equiv \alpha \rho_v u_v + (1-\alpha) \rho_\ell \vec{u}_\ell \end{aligned}$$

respectively. The energy, e , consists of both internal thermal energy, i , and kinetic energy ($e = i + u^2/2$).

The associated integral balance laws for these quantities are written as:

$$\frac{\partial}{\partial t} \int_V \rho dV + \int_A \rho (\vec{u} \cdot \vec{n}) dA = 0 \quad (2.3)$$

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \rho e dV + \int_A \rho e (\vec{u} \cdot \vec{n}) dA = \int_V [\rho (\vec{f} \cdot \vec{u}) + \rho r] dV + \\ \int_A [(\vec{T} \cdot \vec{u}) - \vec{q}] \cdot \vec{n} dA \end{aligned} \quad (2.4)$$

$$\frac{\partial}{\partial t} \int_V \rho \vec{u} dV + \int_A \rho \vec{u} (\vec{u} \cdot \vec{n}) dA = \int_V \rho \vec{f} dV + \int_A (\vec{T} \cdot \vec{n}) dA \quad (2.5)$$

where $\vec{f}$ is the sum of all body forces acting on the fluid and r is the rate of internal heat generation per unit mass from all sources. The surface stress is denoted by the tensor $\vec{T}$ and the heat flux vector by $\vec{q}$.

Each of the three equations (2.3 through 2.5) represents the combination of two similar equations for the individual phases. By retaining the six separate equations and adding an equation of state for each phase, one could solve for the local velocity, density and energy of each phase as well as the local mixture composition and pressure. This would, however, require detailed information about phase interactions and the configuration of the interface that currently can be only roughly estimated, except for a few special cases.

At the expense of some generality, it is much more convenient in many applications to specify the motion of one of the phases with respect to the other or to the mixture. If thermal phase equilibrium is then assumed, only three mixture conservation equations and one mixture equation of state are required to treat separated two-phase flow if the relative

velocity is specified via a correlation for slip ratio, drift velocity or a void-quality function. One additional equation is required for each phase that is allowed to depart from saturation. Mixture equations are not necessarily limited to homogeneous equilibrium flows.

Integral balance laws (2.3) through (2.5) for mass energy and momentum have been written for a single component two-phase mixture with the phases in thermodynamic equilibrium. Since the intended applications of COBRA are for low speed flow with significant surface heat transfer, the following additional assumptions apply.

- Kinetic energy changes are small compared to internal thermal energy changes.
- Work done by body forces and shear stress is considered to be insignificant.
- Internal heat generation in the fluid is ignored.
- Gravity is the only significant body force.

Since the surface, A , of the control volume, V , is assumed to consist of both solid wall and fluid components, it is convenient to split the surface integrals in the balance equations into two components. For an arbitrary surface flux, $\vec{Q}$, the relation is

$$\int_A (\vec{Q} \cdot \vec{n}) dA = \int_W (\vec{Q}_W \cdot \vec{n}) dA + \int_F (\vec{Q}_F \cdot \vec{n}) dA \quad (2.6)$$

where W represents the solid wall portion and F represents the fluid part of A .

Under the assumption above, the only surface integrals of interest over the solid wall are the heat transfer and surface forces. It is understood that advection is allowed only across

the fluid boundary. The fluid and solid components of the surface heat transfer integral will be represented by the Fourier law and the product of an empirical surface heat transfer coefficient, H and temperature difference, respectively. That is,

$$\int_A (\vec{q} \cdot \vec{n}) dA = - \int_F K (\vec{\nabla} T \cdot \vec{n}) dA + \int_W H (T_W - T_F) dA \quad (2.7)$$

where K is the fluid thermal conductivity, T_F is an appropriate local fluid temperature and T_W is the temperature of the solid boundary.

The stress tensor, $\vec{T}$, can be written as the sum of a hydrostatic component, p , and a viscous stress tensor, $\vec{\pi}$, as follows:

$$\int_A (\vec{T} \cdot \vec{n}) dA = - \int_A p \vec{n} dA + \int_A (\vec{\pi} \cdot \vec{n}) dA \quad (2.8)$$

The fluid and solid components of the surface stress integral, Equation (2.8), are

$$\int_A (\vec{T} \cdot \vec{n}) dA = - \int_F p \vec{n} dA + \int_F (\vec{\pi} \cdot \vec{n}) dA + \left\{ - \int_W p \vec{n} dA + \int_W (\vec{\pi} \cdot \vec{n}) dA \right\} \quad (2.9)$$

The wall component, in brackets above, will later be modeled by empirical friction factor and drag coefficient correlations in the momentum equation. Since the work done by shear stresses has been assumed to be negligible in the energy equation, the definition (2.8) results in

$$\int_A \vec{T} \cdot (\vec{u} \cdot \vec{n}) dA = - \int_F p (\vec{u} \cdot \vec{n}) dA \quad (2.10)$$

The left side of Equation (2.10) is combined with the internal energy, i , by defining the enthalpy, h , as $\rho h \equiv \rho i + p$. The resulting temporal derivative of the pressure can be ignored for low-speed flows.

When the preceding assumptions and definitions are applied to the original integral balances, Equations (2.3) through (2.5), the following equations are formed.

Mass

$$\frac{\partial}{\partial t} \int_V \rho dV + \int_F \rho (\vec{u} \cdot \vec{n}) dA = 0 \quad (2.11)$$

Energy

$$\frac{\partial}{\partial t} \int_V \rho h dV + \int_F \rho h (\vec{u} \cdot \vec{n}) dA = - \int_F K (\vec{\nabla} T \cdot \vec{n}) dA + \int_W H (T_W - T_F) dA \quad (2.12)$$

Momentum

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \rho \vec{u} dV + \int_F \rho \vec{u} (\vec{u} \cdot \vec{n}) dA &= \int_V \rho \vec{g} dV - \int_F p \vec{n} dA + \int_F (\vec{\pi} \cdot \vec{n}) dA \\ &- \int_W p \vec{n} dA + \int_W (\vec{\pi} \cdot \vec{n}) dA \end{aligned} \quad (2.13)$$

In Section 2.2, these integral balance equations will be applied to rod-bundle geometry typical of a nuclear reactor core. The constraints imposed by this geometry generate a system of subchannel partial differential equations for which solutions will be derived in succeeding sections.

2.2 SUBCHANNEL EQUATIONS

In a nuclear reactor core, fluid flow is constrained by the surfaces of closely spaced fuel rods oriented parallel to the primary axial flow direction. On a small scale, the fuel rods partition the flow area into many small subchannels which communicate laterally through narrow gaps. Since it would be impractical to attempt a detailed resolution of the flow field within a subchannel, the appropriate volume for the preceding conservation equations is a section of a full subchannel as illustrated in Figure 2-1.

It is assumed that any lateral flow is directed by the gap through which it flows and loses its sense of direction after leaving the gap region. This assumption provides the character of the so-called subchannel equation system. It allows subchannels to be connected arbitrarily since no fixed lateral coordinate is required. A fully three-dimensional physical situation may be represented with relative ease simply by connecting channels in a three-dimensional array. Since crossflow may exist only between two adjacent channels, no specific lateral boundary conditions are required.

Because the spatial orientation of each crossflow is fixed by its associated gap, a convention must be adopted to define the positive direction for each crossflow. Given two

FIGURE 2-1. Relation of Subchannel Control Volume to Reactor Core

adjacent channels, i and j , separated by a gap, k , the cross-flow w_k will be considered positive if the flow is from i to j and negative if from j to i when j is greater than i .

When all N_k gap connections between N_c channels in a particular problem are considered this sign convention can be conveniently incorporated in a symmetric N_k by N_c matrix operator, $[D_c]$, which performs the difference operation across each connection. It happens also that the transpose, $[D_c^T]$, performs the directed summing operation on gap connections around each channel arising when the surface flux integrals in Equations (2.11) through (2.13) are applied to the subchannel control volume in Figure 2-1.

To illustrate the utility of the subchannel ordering matrix, consider lateral fluid heat conduction through the gaps ℓ and m between adjacent subchannels i , j and k as shown in Figure 2-2. The rate of heat conduction, q_k , out of channel i through gap ℓ can be related to the average temperature in each channel by

$$q_\ell = C_\ell (T_i - T_j) \quad (2.14)$$

Similarly, for gap m

$$q_m = C_m (T_j - T_k) \quad (2.15)$$

where C_k is a constant function of the fluid conductivity and gap dimensions. The total heat gained by channel j is the sum of the heat conducted through gaps ℓ and m . Using Equations (2.14) and (2.15),

$$Q_j = C_\ell (T_i - T_j) + C_m (T_j - T_k) \quad (2.16)$$

FIGURE 2-2. Lateral Heat Conduction Problem

Equation (2.16) can be written in a compact general form by using $[D_c]$ to form the temperature difference and the transpose to form the sum. In index notation, Equation (2.16) becomes

$$\{Q_j\} = [D_c^T]_{jk} [C]_{k\ell} [D_c]_{\ell m} \{T_m\} \quad (2.17)$$

where $[C_{kl}]$ is a diagonal matrix of the conduction coefficients. In this three-channel example, the elements of the matrices are defined as

$$[D_c] = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix} \quad [D_c^T] = \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{bmatrix} \quad (2.18)$$

The same logic can be applied to connections between fuel rods and channels and to connections between thermally conducting walls and channels. For N_r fuel rods and N_w walls with N_{kr} and N_{kw} rod-to-channel and wall-to-channel connections, respectively, two additional matrix operators are defined: $[D_r]$ which has dimensions N_{kr} by $(N_c + N_r)$ and $[D_w]$ which is N_{kw} by $(N_c + N_w)$. These will be used later to express the heat transfer between walls, fuel rods and channels as was done in the preceding illustration. The elements of $[D_c]$, $[D_r]$ and $[D_w]$ are listed in the appendix for a somewhat more complicated geometry to more clearly illustrate their meaning.

The matrix operators above are defined on the entire array of rods, walls, channels and their connections. However, in the succeeding derivations it will often be necessary to consider only one channel, wall or gap for clarity. In these cases a vector operator notation will be used to refer only to the summing or differencing operation around the particular element of interest. For example, in the continuity equation (2.19),

$$A \frac{\partial \rho}{\partial t} + \frac{\partial m}{\partial X} + \{D_C^T\}\{w\} = 0 \quad (2.19)$$

the $\{D_C^T\}$ vector sums crossflows around a single channel. In cases where the entire array is intended, matrix notation will be employed. In this case, Equation (2.19) would be written as

$$[A] \frac{\partial \{\rho\}}{\partial t} + \frac{\partial \{m\}}{\partial X} + [D_C^T]\{w\} = 0 \quad (2.20)$$

where $[A]$ is a diagonal N_C by N_C matrix and $\{\rho\}$, $\{m\}$, and $\{w\}$ are vectors of density, mass flow rate, and crossflow, respectively.

At the beginning of this section, it was assumed that sufficient space and time averaging had been performed to provide continuous derivatives throughout the flow field. However, to solve the integral balance equations it is necessary to define volume and surface averaged quantities over the entire control volume. Using the density and the axial mass flux as examples, the volume and surface averages are defined, respectively, as:

$$\langle\langle\rho\rangle\rangle_V \equiv \frac{1}{V} \int_V \rho dV \quad (2.21)$$

$$\langle\rho u\rangle_A \equiv \frac{1}{A} \int_A \rho (u \cdot n) dA \quad (2.22)$$

where $V = \int_V dV$ and $A = \int_A dA$. These definitions imply no additional assumptions about the behavior of the individual phases since they are merely an alternate method of representing the integrals.

The integral balances in Equations (2.11) through (2.13) will now be applied to the control volume in Figure 2-3 using the lateral connection matrices and definitions (2.21) and (2.22). Empirical correlations as described in Section 5 will be utilized where necessary to close the set. The result will be a system of subchannel differential equations for which solution methods will be described in Section 3.

Consider the subchannel section in Figure 2-3 that defines the control volume for the integral Equations (2.11) through (2.13). The centroid of the control volume is located at X and its length is ΔX . This places the upper and lower surfaces at $X + (\Delta X/2)$ and $X - (\Delta X/2)$, respectively. The axial

FIGURE 2-3. Subchannel Control Volume

flow area at these surfaces is denoted by A and the axial velocity by u . Assuming a linear variation in axial area between the upper and lower surfaces, the volume, V , is numerically equivalent to $\bar{A}\Delta X$ where $\bar{A}$ is the average axial flow area in V .

The lateral flow areas lie in the gap space between fuel rods on planes connecting fuel rod centerlines. The width of the gap is S and the lateral velocity is v . There is an arbitrary number of lateral flow areas (three in the case of Figure 2-3) and the gap width, S , may vary from gap to gap. The area of each lateral surface is $S\Delta X$.

2.2.1 Mass Balance

Equation (2.11) may be applied directly to the subchannel control volume. The transposed connection vector $\{D_C^T\}$, forms the lateral component of the mass flux integral.

$$V \frac{\partial}{\partial t} \langle \rho \rangle_V + \langle \rho u \rangle_A A \Big|_{X+\frac{\Delta X}{2}} - \langle \rho u \rangle_A A \Big|_{X-\frac{\Delta X}{2}} + \{D_C^T\} \langle \rho v \rangle_S S \Delta X = 0 \quad (2.23)$$

where the area averaged lateral mass flux is defined by

$$\langle \rho v \rangle_S = \frac{1}{S\Delta X} \int_{A=S\Delta X} \rho (\vec{u} \cdot \vec{n}) dA \quad (2.24)$$

The subchannel equation is formed by dividing Equation (2.23) by ΔX and taking the limit as ΔX becomes small:

$$A \frac{\partial}{\partial t} \langle \rho \rangle_V + \frac{\partial}{\partial X} \langle \rho u \rangle_A A + \{D_C^T\} \langle \rho v \rangle_S S = 0 \quad (2.25)$$

It is not meaningful or necessary to attempt forming partial derivatives in the lateral directions because the shape of the control volume is constrained by the fixed fuel rod boundaries.

The division by ΔX references the equation to changes in mass per unit axial channel length. The first term is the time rate of change of mass per unit axial length and the second is the spatial variation in axial mass flow rate per unit length. The last term is the sum on all gap connections of the lateral mass flow rate per unit length which is the "diversion crossflow mixing" or "crossflow" associated with subchannel analysis. Both the axial and lateral flow terms are derived from an area averaged mass flux and are of equal importance to the flow solution. It is not necessary to assume that the crossflow be small with respect to the axial flow unless the specific solution method requires it.

2.2.2 Energy Balance

The procedure used to apply the integral energy balance, (2.12), to the subchannel control volume is the same as that employed in constructing the continuity equation, (2.25), except that further definitions must be made to describe the surface heat transfer and lateral fluid heat conduction.

The surface area of a fuel rod in the control volume, V , is the product of the length increment, ΔX , and the fraction, Φ , of its total perimeter, P_r , facing V . Similarly the surface area of a conducting wall in V is the product of ΔX and the length L_w of the wall facing V . A typical arrangement is shown in Figure 2-4.

The area averages for the surface heat fluxes from fuel rods and walls could be defined in the same way as the area averages for the convective fluxes. However, most commonly

FIGURE 2-4. Rod and Wall Surface Heat Transfer Geometry

used surface heat transfer correlations already imply considerable surface averaging and require a bulk fluid temperature. Therefore, it is quite appropriate to dispense with formal averaging and use the rod and wall-to-channel connection matrices to compute the surface heat transfer to the control volume. The total heat input to V from rods is

$$Q_r = \Delta x \{D_r^T\} [P\Phi H] [D_r] \{T\} \quad (2.26)$$

From walls, the equivalent expression is

$$Q_w = \Delta x \{D_w^T\} [LH] [D_w] \{T\} \quad (2.27)$$

where H is the surface heat transfer coefficient. The product $[D_r] \{T\}$ forms a difference between the rod surface temperature and bulk channel temperature. The $[D_w] \{T\}$ product is similarly defined.

Consider lateral fluid heat conduction through the gap between two channels, i and j , as illustrated in Figure 2-5. The total rate of heat conduction, Q_c , through the gap surface, S , can be determined exactly via the Fourier law as

FIGURE 2-5. Lateral Fluid Heat Conduction Geometry

$$Q_c = -S\Delta X \left\langle k \frac{\partial T}{\partial y} \right\rangle_S \quad (2.28)$$

where k is the fluid conductivity and the partial derivative indicates the lateral temperature gradient in the gap.

Because the local lateral temperature gradient in this complex geometry is not readily available, the heat conduction rate must be related to the bulk fluid temperature of the two adjacent channels. This leads to a finite difference form using the channel centroid separation distance, L_c , and an empirical correction factor, C . The temperature difference is formed by the channel connection matrix. As in Equation (2.22), the resulting expression for the total energy input to V by lateral conduction is

$$Q_c = -\Delta X \{D_c^T\} \left[\frac{SC \langle k \rangle}{L_c} \right] [D_c] \{T\} \quad (2.29)$$

The turbulent mixing model of COBRA-IIIC is used to account for lateral turbulent energy exchange (mixing). A fluctuating crossflow per unit length, w' , is assumed which performs an equal mass exchange between adjacent channels. The relationship between w' and diffusivity is discussed in

Section 5.4. Using the subchannel ordering matrices, the total turbulent energy input to V, Q_T , can be expressed as

$$Q_T = -\Delta X \{D_C^T\} [w'] [D_C] \{h'\} \quad (2.30)$$

where h' is the enthalpy transported by the turbulent cross-flow. Axial turbulent energy mixing is ignored. The same model will be used in the next subsection to account for turbulent momentum mixing.

As with the preceding continuity equation, all the above contributions to the total energy change in the control volume are summed and divided by ΔX . In the limit as ΔX approaches zero, the result becomes the subchannel energy equation:

$$\begin{aligned} A \frac{\partial}{\partial t} \langle \rho h \rangle_V + \frac{\partial}{\partial X} \langle \rho u h \rangle_A + \{D_C^T\} \{ \langle \rho v h \rangle_S \} = \\ \{D_r^T\} [P \Phi H] [D_r] \{T\} + \{D_w^T\}^T [LH] [D_w] \{T\} + \\ \frac{\partial}{\partial X} A \left\langle k \frac{\partial T}{\partial X} \right\rangle_A - \{D_C^T\} \left[\frac{SC \langle k \rangle}{L_C} \right] [D_C] \{T\} - \{D_C^T\} [w'] [D_C] \{h'\} \end{aligned} \quad (2.31)$$

Correlations for the heat transfer coefficients, geometry factors and turbulent mixing must be specified by code users. Several correlations incorporated in the code may be selected via input. If other correlations are desired, it is relatively easy to adapt the code to include them.

2.2.3 Axial Momentum Balance

Two components of momentum must be considered: an axial component, $\langle \rho u \rangle_A$ and a lateral, gap-directed component, $\langle \rho v \rangle_S$.

The balance equation for the axial component will be discussed first and the lateral component, which requires a modified control volume, will follow.

The axial momentum equation is formed by applying the integral momentum balance, Equation (2.13), to the subchannel control volume, considering only the axial component of momentum, $\langle pu \rangle$. Descriptions of the pressure and shear forces on the control volume and the turbulent momentum mixing are required.

Using the area average, the net axial pressure force, F_p , acting on the ends of the control volume is

$$F_p = -\langle p \rangle_A A \Big|_{x+\frac{\Delta X}{2}} + \langle p \rangle_A A \Big|_{x-\frac{\Delta X}{2}} \quad (2.32)$$

If the area varies axially, an additional force, F_w , is exerted by the side walls. The axial area variation is assumed to be linear within ΔX and, if the pressure also varies linearly within ΔX , this force can be expressed as

$$F_w = \langle p \rangle_X \left(A_{x+\frac{\Delta X}{2}} - A_{x-\frac{\Delta X}{2}} \right) \quad (2.33)$$

The total pressure force on the control volume is the sum of F_p and F_w which, after factoring Equation (2.32), can be written as

$$F_w + F_p = -A_X \left[\langle p \rangle_{x+\frac{\Delta X}{2}} - \langle p \rangle_{x-\frac{\Delta X}{2}} \right] \quad (2.34)$$

The remainder of the solid surface stress integral in Equation (2.13) is approximated by empirical wall friction correlations and form loss coefficients. An axial drag force, F_D , proportional to the axial momentum flux, is computed:

$$F_D = \frac{1}{2} [f \Delta X P_w + K A] \langle \rho u^2 \rangle_A \quad (2.35)$$

where f is a dimensionless friction factor determined by correlation, P_w is the wetted perimeter of the channel, and K is the total form loss coefficient in Δx . The standard definition of hydraulic diameter, D_h , is applied so that

$$F_D = \frac{1}{2} \left(\frac{f' \Delta X}{D_h} + K \right) \langle \rho u^2 \rangle_A A \quad (2.36)$$

where $f' = 4f$.

At the present time, the fluid-to-fluid viscous shear stress (momentum diffusion) between channels is ignored as small in comparison to the wall shear forces. The turbulent momentum mixing between channels is modeled in the same way as the thermal energy mixing term, Equation (2.30). The total axial force on the control volume due to turbulent mixing, F_m , is computed with the connection matrices

$$F_m = -C_T \Delta X \{D_c^T\} [w'] [D_c] \{u'\} \quad (2.37)$$

where u' is the axial velocity transported by the turbulent crossflow and C_T is a constant correction factor to account for the imperfect analogy between turbulent transport of thermal energy and momentum.

The subchannel balance for axial momentum is obtained as before using the above definitions. The result is

$$\begin{aligned} \frac{\partial}{\partial t} \langle \rho u \rangle_V A + \frac{\partial}{\partial X} \langle \rho u^2 \rangle_A A + \{D_C^T\} \langle \rho u v \rangle_S S = \\ -A \frac{\partial}{\partial X} \langle p \rangle_A - \frac{1}{2} \left(\frac{f'}{D_h} + \frac{K}{\Delta X} \right) \langle \rho u^2 \rangle_A A - A \langle \rho \rangle_V \cos \theta - \\ C_T \{D_C^T\} [w'] [D_C] \{u'\} \end{aligned} \quad (2.38)$$

where θ is the channel axis orientation angle measured from the vertical.

2.2.4 Lateral Momentum Balance

For the lateral momentum component, it has been assumed that the flow direction is determined by the gap orientation and that the crossflow loses its identity away from the gap. Therefore, Equation (2.13) need only be integrated in the region of the influence of each gap. This requires a modified control volume centered in the gap, illustrated in Figure 2-6.

FIGURE 2-6. Control Volume for Lateral Momentum

The modified control volume, V' , is bounded laterally by the fuel rod surfaces and by planes, G , joining the adjacent channel centroids and the fuel rod centerlines. The upper and lower surfaces of V' are closed by the flow area, A' . Note that V' and the original subchannel control volume, V , overlap so that the sum of all V' is equal to the sum of all V over the entire bundle. It is convenient to define a lateral pseudolength, ℓ , such that

$$S\ell = A' \quad (2.39)$$

where S is the gap width. The length, ℓ , is approximately the distance between adjacent channel centroids.

The complex geometry of the gap in the direction of the crossflow precludes the exact calculation of wall friction and drag forces, lateral momentum flux and the lateral pressure forces. These quantities must be determined from empirical correlation or approximated by various means. The assumptions necessary to define these terms are based on a rod bundle configuration but the resulting forms may be applied to other situations equally well if the various adjustable coefficients are computed judiciously.

The pressure loss through the gap is modeled by an overall loss coefficient, K_G , which accounts for friction as well as the form drag caused by the area change. The total drag force, F_d , acting on the control volume is

$$F_d = \frac{1}{2}K_G \langle \rho v^2 \rangle_S S \Delta X \quad (2.40)$$

In rod bundles, K_G is on the order of 0.5. Neither fluid shear nor turbulent momentum diffusion is explicitly considered in the lateral direction.

The main driving force for crossflow is the pressure imbalance between adjacent channels. For two adjacent channels, i and j , the total pressure force, F_p , on V' would be given by

$$F_p = \left[\langle p \rangle_G|_i - \langle p \rangle_G|_j \right] S\Delta X \quad (2.41)$$

The area is chosen as $S\Delta X$ to be consistent with the definition of the drag coefficient in Equation (2.40). As ΔX becomes small, the average pressure over the surfaces, G , can be closely approximated by the subchannel area averaged pressure $\langle p \rangle_A$. Using the connection matrix, Equation (2.39) becomes

$$F_p = S\Delta X \{D_c\} \{\langle p \rangle_A\} \quad (2.42)$$

Although it was assumed that the crossflow is defined only in and near its gap region, it is also recognized that the crossflows are not completely independent of each other. The lateral momentum flux through one gap may affect the next gap downstream, particularly in square arrays. It is possible to write an approximation for the lateral momentum flux term if each gap is assigned a direction angle, β , from some arbitrary reference. Any gaps communicating with either of the two channels adjacent to the gap of interest may have a contribution, depending on their orientation. The gap reference angles are illustrated in Figure 2-7.

FIGURE 2-7. Gap Reference Angles

With these definitions, then, the net lateral momentum flux, G_s , out of V' is approximated by

$$G_s = C_s \{D_c\} [D_c^T] \{ (N) \langle \rho v^2 \rangle_s \Delta X \cos \Delta\beta \} \quad (2.43)$$

The factor C_s is included to help account for the imperfect coupling between communicating gaps and should have a value less than unity. The binary operator (N) is -1 if positive crossflow is out of one of the two channels i or j in Figure 2-7 and +1 if positive crossflow is inward. The angle $\Delta\beta$ is the difference between the reference angle of a communicating gap and the gap of interest.

If Equation (2.43) is applied to two-dimensional slab geometry, the connection matrices form a centered finite difference, which may cause some instability in the solution. For this reason, and because of lack of information on the factor K_s , this term was made optional in COBRA. Although it will be carried through subsequent derivations, its effects should be evaluated carefully against experimental data before it is used.

The reference angles, β , also provide a means of computing a lateral gravity force, F_g , for inclined bundles. If the reference direction for β is chosen parallel to the plane described by the bundle axis and the vertical, the gravity force on V' is

$$F_g = -\langle\langle\rho\rangle\rangle_V S \Delta X \sin\theta \cos\beta \quad (2.44)$$

where θ is the axial orientation of the bundle measured from vertical. This term is not yet available in COBRA, but is included in this document for completeness.

The lateral momentum balance can now be formed by adding the momentum fluxes and equating them to the summation of forces:

$$\begin{aligned} S \Delta X \frac{\partial}{\partial t} \langle\langle\rho v\rangle\rangle_V + S \ell \langle\rho v u\rangle_A \Big|_{X+\frac{\Delta X}{2}} - S \ell \langle\rho v u\rangle_A \Big|_{X-\frac{\Delta X}{2}} + \\ C_S \{D_C\} [D_C^T] \{ (N) \langle\rho v^2\rangle_S S \Delta X \cos\Delta\beta \} = -\frac{1}{2} K_G \langle\rho v^2\rangle_S S \Delta X + \\ S \Delta X \{D_C\} \{ \langle p \rangle_A \} - \langle\langle\rho\rangle\rangle_V S \Delta X \sin\theta \cos\beta \end{aligned} \quad (2.45)$$

Dividing Equation (2.45) by $\ell \Delta X$ and taking the limit as ΔX approaches zero yields the subchannel differential equation for crossflow:

$$\begin{aligned} \frac{\partial}{\partial t} \langle\langle\rho v\rangle\rangle_{V,S} + \frac{\partial}{\partial X} \langle\rho v u\rangle_{A,S} + C_S \{D_C\} [D_C^T] \{ (N) \frac{S}{\ell} \langle\rho v^2\rangle_S \cos\Delta\beta \} = \\ \frac{S}{\ell} \{D_C\} \{ \langle p \rangle_A \} - \frac{1}{2} \frac{S}{\ell} K_G \langle\rho v^2\rangle_S - \langle\langle\rho\rangle\rangle_{V,S} \sin\theta \cos\beta \end{aligned} \quad (2.46)$$

To illustrate the character of the subchannel momentum equations, the momentum transport terms of Equations (2.38) and (2.46) are compared to the classical Cartesian components of $\nabla \cdot \rho \vec{u} \vec{u}$ in Table 2-1. Assuming that the lateral momentum flux diagonal term is modeled correctly, it can be seen that the only terms missing from a fully three-dimensional system are the lateral cross products of velocity. The absence of these two terms makes it impossible for COBRA to consider complex three-dimensional circulation. However, they would be negligible in the center of a rod bundle and quite accurate simulations of three dimensional phenomena can be achieved in that geometry.

TABLE 2-1. Comparison of Classical and Subchannel
Momentum Transport

<u>x Component</u>		
$\frac{\partial}{\partial x} \rho u^2$	$+ \frac{\partial}{\partial y} \rho uv$	$+ \frac{\partial}{\partial z} \rho uw$
$\frac{\partial}{\partial x} \langle \rho u^2 \rangle_A$	$+ [D_C^T] \{ \langle \rho uv \rangle_S \}$	
<u>y Component</u>		
$\frac{\partial}{\partial x} \rho vu$	$+ \frac{\partial}{\partial y} \rho v^2$	$+ \frac{\partial}{\partial z} \rho vw$
$\frac{\partial}{\partial x} \langle \rho vu \rangle_A$	$+ C_S \{ D_C \} [D_C^T] \{ (N) \langle \rho v^2 \rangle_S \cos \Delta \beta \}$	-----
<u>z Component</u>		
$\frac{\partial}{\partial x} \rho wu$	$+ \frac{\partial}{\partial y} \rho wv$	$+ \frac{\partial}{\partial z} \rho w^2$
$\frac{\partial}{\partial x} \langle \rho wu \rangle_A$	-----	$+ C_S \{ D_C \} [D_C^T] \{ (N) \langle \rho v^2 \rangle_S \cos \Delta \beta \}$
		Classical
		Subchannel

3.0 NUMERICAL SOLUTION

Two solution techniques are used in COBRA to solve the preceding system of subchannel equations. One is an implicit technique very similar to that used in the COBRA-IIIC code (Rowe, 1973). It provides a direct solution for the steady state and has limited transient capability but is restricted to cases where axial flow is positive and generally greater than the lateral flows. The other solution procedure removes the positive flow restriction by use of an explicit technique which is limited to small time steps. The explicit procedure is used exclusively for transient problems but it can accept a steady-state solution from the implicit method as an initial condition. In many cases, such as a steady recirculation, the explicit method can be used to provide a transient solution approaching a steady-state condition that could not be solved implicitly.

The implicit procedure currently has several features not available in the explicit solution. Two-phase slip models are available along with several options for the void-quality relation and two-phase friction multiplier in the axial direction. A wire wrap spacer model is also available, and specifies the lateral flow where wire wraps cross a gap as a function of the wrap pitch and axial flow rate. This model is similar to the COBRA-IIIC wire wrap model except that the numerics are more efficient.

The explicit solution currently uses only the homogeneous equilibrium model for two-phase flow. However, development underway will provide the capability to consider both axial and lateral relative phase motion by use of the drift flux concept. A technique has been developed to calculate the motion of density gradients approaching liquid-vapor interface conditions stably and accurately with this homogeneous model.

Both solution methods employ the same models to simulate the fuel rods and conducting walls. The fuel conduction model, developed by Cena et al. (1975), uses the method of weighted residuals by the orthogonal collocation technique (Finlayson, 1972). A Kirchoff transformation is employed so that temperature-dependent thermal conductivity may be considered. The details of the fuel model derivation are described in Section 4.

The fuel is interfaced with the fluid thermal-hydraulic solution by means of a surface heat transfer coefficient for which a correlation may be specified via code input. A modified version of the RELAP-IV heat transfer correlation package is also available (Moore and Rettig, 1973). The details of these correlations and other constitutive relations are discussed in Section 5.

The reference pressure approach is used in both flow solutions. The local fluid density is assumed to be a function of the local enthalpy and a spatially uniform reference pressure. Thus local momentum effects or hydrostatic head do not enter fluid property calculations. This assumption is valid as long as these spatial pressure variations are small compared to the system pressure.

To solve the four subchannel equations derived in the preceding section, as well as the state equation, the area and volume averaged terms must be related so that the equations can be recast in terms of five primary variables. These are axial mass flow rate, m , lateral mass flow rate per unit axial length (crossflow), w , mixture static enthalpy, h , or flowing enthalpy, $\hat{h}$, mixture density, ρ , and pressure, P . The definitions necessary to form these primary variables are different for the two solution methods since the implicit solution is formed in terms of flowing quality and allows

slip while the explicit solution requires static quality and does not allow slip. These definitions are listed in Table 3-1. Whenever applicable in later sections, a more detailed derivation will be shown when the specific definition is first used.

TABLE 3-1. Definition of Variables

Symbol	Description and Units	Definition
m	Axial mass flow rate, (lb/sec)	$m = \langle \rho u \rangle A$
w	Lateral mass flow per unit length (crossflow), (lb/sec-ft)	$w = \langle \rho v \rangle S$
w'	Turbulent crossflow per unit length, (lb/sec-ft)	
ρ	Mixture density, (lb/ft ³)	$\rho = \langle \langle \rho \rangle \rangle v + (1-\alpha) \rho_l$
$\hat{\rho}$	Two-phase momentum density, (lb/ft ³)	$\hat{\rho} = \frac{\langle \rho u \rangle^2}{\langle \rho u^2 \rangle}$
	In terms of void-quality	$\frac{1}{\hat{\rho}} = \frac{(1-\hat{x})^2}{\rho_l(1-\alpha)} + \frac{\hat{x}^2}{\rho_v \alpha}$
$\hat{v}$	Momentum specific volume, (ft ³ /lb)	$\hat{v} = \frac{1}{\hat{\rho}}$
v	Mixture specific volume, (ft ³ /lb)	$v = 1/\rho$
	In terms of static quality	$v = xv_v + (1-x)v_l$
h	Mixture enthalpy, (Btu/lb)	$h = \frac{\langle \langle \rho h \rangle \rangle}{\langle \langle \rho \rangle \rangle}$
	In terms of static quality	$h = xh_v + (1-x)h_l$
h'	Enthalpy transported by the turbulent crossflow, (Btu/lb)	
$\hat{h}$	Flowing enthalpy, (Btu/lb)	$\hat{h} = \langle \rho u h \rangle / \langle \rho u \rangle$
	In terms of flowing quality	$\hat{h} = \hat{x}h_v + (1-\hat{x})h_l$
$\hat{x}$	Flowing quality	$\hat{x} = \langle \alpha \rho_v u_v \rangle / m$
x	Static quality (vapor mass fraction)	$x = \langle \langle \alpha \rho_v \rangle \rangle / \rho$
ψ	Function defining relationship between h and $\hat{h}$, (lb/ft ³)	$\psi = \rho_l x(1-\alpha) - \rho_v \alpha(1-x)$
		$\psi = (\hat{h}-h)\rho/(h_v-h_l)$
α	Vapor volume fraction	$\alpha = (\rho_l - \rho)/(\rho_l - \rho_v)$
u	Axial velocity, (ft/sec)	$u = \langle \rho u \rangle / \rho = m/\rho A$
$\hat{u}$	Momentum velocity, (ft/sec)	$\hat{u} = m\hat{v}/A = \langle \rho u^2 \rangle / \langle \rho u \rangle$
u'	Axial velocity transported by the turbulent crossflow, (ft/sec)	
P	Pressure, (lb _f /ft ²)	$P = P_v = P_l$
v	Lateral velocity, (ft/sec)	$v = \langle \rho v \rangle / \rho = w/\rho S$
A	Subchannel flow area, (ft ²)	
S	Gap width, (ft)	

3.1 IMPLICIT SOLUTION

The implicit numerical flow solution in COBRA-IV is basically the same as that used in previous versions of COBRA. It is limited to problems in which the axial flow rate is positive and greater than the transverse flow rate at all locations.

Two-phase slip flow is considered with the assumption that the phases are in thermal equilibrium and that the phase velocities and volume fractions are uniformly distributed within the control volume. With the reference pressure equation of state, thermal equilibrium implies spatially uniform saturation properties.

Lateral phase slip is treated identically to axial slip to be consistent with the assumption of uniform phase velocities and distribution. This implies that the quality of the fluid transported laterally is the same as that of the fluid transported axially, allowing the same definition of flowing enthalpy and quality to apply in both lateral and axial advection. That is, the flowing enthalpy is defined as

$$\hat{h} \equiv \frac{\langle \rho u h \rangle}{\langle \rho u \rangle} = \frac{\langle \rho v h \rangle}{\langle \rho v \rangle} \quad (3.1)$$

Similarly, the definition of flowing quality is

$$\hat{x} \equiv \frac{\langle \alpha \rho_v u_v \rangle}{\langle \rho u \rangle} = \frac{\langle \alpha \rho_v v_v \rangle}{\langle \rho v \rangle} \quad (3.2)$$

A further consequence of assumption of uniform phase distribution is that the area averaged mass flux must be equivalent to the volume averaged mass flux in both directions. That is,

and

$$\begin{aligned} m &\equiv A\langle \rho u \rangle = A\langle\langle \rho u \rangle\rangle \\ w &\equiv S\langle \rho v \rangle = S\langle\langle \rho v \rangle\rangle \end{aligned} \quad (3.3)$$

It is important to note here that the flowing enthalpy, $\hat{h}$, is not equivalent to the volume averaged static enthalpy, h , because the phase velocities are allowed to differ.

The above relations and assumptions will now be applied to restate the subchannel equations of the previous section in a soluble form. The continuity equation (2.25) can be rewritten directly in terms of ρ , m and w as

$$A \frac{\partial}{\partial t} \rho + \frac{\partial}{\partial X} m + \{D_C^T\}\{w\} = 0 \quad (3.4)$$

Using the definition of flowing enthalpy, the energy equation becomes

$$A \frac{\partial}{\partial t} \rho h + \frac{\partial}{\partial X} m \hat{h} + \{D_C^T\}\{w \hat{h}\} = Q \quad (3.5)$$

where Q contains the terms on the right-hand side of Equation (2.31). Factoring Equation (3.5) and applying continuity yields

$$A \left(\frac{\partial}{\partial t} \rho (h - \hat{h}) + \rho \frac{\partial \hat{h}}{\partial t} \right) + m \frac{\partial \hat{h}}{\partial X} + \{D_C^T\}\{w \hat{h}\} - \hat{h} \{D_C^T\}\{w\} = Q \quad (3.6)$$

The static enthalpy, h , and flowing enthalpy, $\hat{h}$, can be related by defining a new property, ψ , introduced by Tong (1965), which is defined as

$$\psi = \rho (\hat{h} - h) / (h_v - h_\ell) \quad (3.7)$$

By substituting the ψ function for $\frac{\partial h}{\partial t}$ and applying the chain rule, the energy equation is stated solely in terms of the flowing enthalpy as

$$A(\rho - h_{fg} \frac{\partial \psi}{\partial h}) \frac{\partial \hat{h}}{\partial t} + m \frac{\partial \hat{h}}{\partial X} + \{D_C^T\}\{\hat{w}\hat{h}\} - \hat{h}\{D_C^T\}\{\hat{w}\} + Q \quad (3.8)$$

The ψ function can be related to the void fraction and flowing quality and consequently to the slip ratio by simply applying the void and quality definitions. Thus

$$\psi = \rho_l \hat{x}(1-\alpha) - \rho_v \alpha(1-\hat{x}) \quad (3.9)$$

The axial momentum equation (2.38) is rewritten by making use of the momentum velocity definition, $\hat{u}$, and the assumption of uniform phase distribution

$$\frac{\partial}{\partial t} m + \frac{\partial}{\partial X} m \hat{u} + \{D_C^T\}\{\hat{w}\hat{u}\} = F \quad (3.10)$$

where F contains all the forces acting on the control volume as given by the right-hand side of Equation (2.38).

Equation (3.10) is modified by applying the definition of $\hat{u}$ the specific volume for momentum, $\hat{v}$, and differentiating the convection term

$$\frac{\partial}{\partial t} m + \frac{\hat{v}}{A} \frac{\partial m^2}{\partial X} + m^2 \frac{\partial}{\partial X} \frac{\hat{v}}{A} + \{D_C^T\}\{\hat{u}\hat{w}\} = F \quad (3.11)$$

The momentum specific volume, $\hat{v}$, is related to the void fraction and flowing quality by

$$\hat{v} = \frac{(1-\hat{x})^2}{\rho_l(1-\alpha)} + \frac{\hat{x}^2}{\rho_v \alpha} \quad (3.12)$$

The second term is differentiated again and the continuity equation is substituted for $\frac{\partial m}{\partial X}$ to give

$$\frac{\partial m}{\partial t} + 2m \frac{\hat{v}}{A} (-A \frac{\partial \rho}{\partial t} - \{D_C^T\}\{w\}) + m^2 \frac{\partial \hat{v}/A}{\partial X} + \{D_C^T\}\{u\hat{W}\} = F \quad (3.13)$$

Similarly the transverse momentum equation (2.46) is written in terms of w , $\hat{u}$ and $\hat{v}$ as

$$\frac{\partial}{\partial t} w + \frac{\partial}{\partial X} \hat{u} w + \frac{C_S}{S^2} \{D_C\} [D_C^T] \{ (N) \frac{S}{L} w^2 \hat{v} \cos \Delta \beta \} = G \quad (3.14)$$

where G represents the right-hand side of Equation (2.46).

Equations (3.4), (3.8), (3.13) and (3.14) are the basic equations from which the implicit numerical scheme is derived. The finite difference analogs and the numerical procedure are discussed in the following sections.

3.1.1 Difference Equations

The partial differential equations derived above apply to a series of discrete, arbitrarily interconnected subchannels. They contain partial derivatives in time and in the axial spatial coordinate parallel to the subchannel axes. By dividing the subchannels into a finite number of axial segments and assigning the main variables specific positions on the resulting computation mesh, the partial derivatives are approximated by finite differences. The spatial locations of the variables on the mesh are illustrated in Figure 3-1. Note that the system is already discretized in the lateral direction by the subchannel geometry. The generalized forms of the finite difference equations are:

Fluid continuity

$$\frac{1}{\Delta t} \bar{A}_j (\rho_j - \rho_j^n) + \frac{m_j - m_{j-1}}{\Delta X} + \{D_C^T\}\{w_j\} \quad (3.15)$$

FIGURE 3-1. Placement of Variables for Implicit Solution

Subchannel energy

$$\begin{aligned}
 & \frac{1}{\Delta t} A_j \left(\rho_j^n - h_{fg} \frac{\partial \psi}{\partial h} \right) (\hat{h}_j - \hat{h}_j^n) + \frac{1}{\Delta X} m_{j-1} (\hat{h}_j - \hat{h}_{j-1}) + \\
 & \{D_C^T\} \{\hat{h}\tilde{w}\}_j - \hat{h}_j \{D_C^T\} \{\tilde{w}_j\} = \{D_R^T\} [P\bar{\theta}\bar{H}] [D_r] \left\{ T_r \right\}_j + \\
 & \frac{1}{\Delta X^2} \left(kA_j (\tilde{T}_{j+1} - \tilde{T}_j) - kA_{j-1} (\tilde{T}_j - \tilde{T}_{j-1}) \right) + \\
 & \{D_W^T\} [LH] [D_w] \left\{ T_w \right\}_j - \{D_C^T\} \left[\frac{CS\bar{k}}{L_C} \right] [D_c] \{T_j\} - \\
 & \{D_C^T\} [w'] [D_c] \{h'_j\}
 \end{aligned} \tag{3.16}$$

Axial momentum

$$\begin{aligned} & \frac{m_j - m_j^n}{\Delta t} - 2\bar{m} \frac{\hat{v}_j}{A_j} \left(A_j \left(\frac{\rho_j - \rho_j^n}{\Delta t} \right) + \{D_C^T\} \{w_j\} \right) + \\ & m_{j-1}^2 \left(\frac{(\hat{v}/A)_j - (\hat{v}/A)_{j-1}}{\Delta X} \right) + \{D_C^T\} \{\hat{u}_j * w_j\} = -\bar{A} \left(\frac{p_j - p_{j-1}}{\Delta X} \right) - \\ & \bar{A} K_L m_j^2 - \{D_C^T\} \{w'\} [D_C] \{u'_j\} - \bar{A} \rho_j \cos \theta \end{aligned} \quad (3.17)$$

Transverse momentum

$$\begin{aligned} & \frac{w_j - w_j^n}{\Delta t} + \frac{\hat{u} * w_j - \hat{u} * w_{j-1}}{\Delta X} + \frac{C_S}{S^2} \{D_C\} [D_C^T] \left\{ (N) \frac{S}{\ell} \frac{w_j^2}{\rho} \cos \Delta \beta \right\} = \\ & \frac{S}{\ell} \{D_C\} \{p_{j-1}\} - \frac{S}{\ell} C_j w_j \end{aligned} \quad (3.18)$$

In the above equations,

$\bar{A}_j$ = average flow area = $0.5 (A_j + A_{j-1})$

$\bar{k}_j$ = average subchannel gap fluid thermal conductivity,
 $0.5 (k_i + k_l)$. i and l refer to adjacent
subchannels.

$\bar{H}$ = rod average heat transfer coefficient $\frac{\sum_{i=1}^n H_i \phi_i}{\sum_{i=1}^n \phi_i}$,

n = number of subchannels adjacent to rod

T = subchannel temperature

T_R = rod surface temperature

T_w = temperature of conducting wall

$\bar{m} = 0.5 (m_j + m_{j-1})$

$$K_L = \frac{v_l f \phi}{2D_h A_j^2} + \frac{K \hat{v}}{2\Delta X A_j^2}$$

$$C_j = \begin{cases} .5 \frac{K_G |\tilde{w}_j|}{\rho^* s^2} & \text{if } |w| \geq .001 \\ .001 & \text{if } |w| < .001 \end{cases}$$

and the superscripts are defined as:

- * = quantity is convected by the associated flow
- n = previous time step (no superscript implies present time)
- ~ = present time but previous iteration.

The time derivatives are approximated by first-order backward differences. All major variables except those actually forming the time difference are assumed to be at the new, current time level and must be solved simultaneously. The equations are thus implicit in time which makes the stability of the numerical solution independent of the time step size. In fact, the steady-state solution is obtained by using a time step of 10^{10} seconds (over 300 years).

First-order backward differences are also used for all spatial first derivatives; upwind (or donor cell) differencing is used exclusively for convective terms. The donor cell definition is implied in the axial direction by the assumption of positive flow. All major variables for each channel at a specific axial level are interrelated by the lateral connection matrices and must be solved simultaneously. The lateral pressure difference is derived by integrating the axial pressure gradient which forces pressure disturbances such as a blockage or nonuniform voiding

to propagate "upstream." This requires an additional, external iteration and makes the set of finite difference equations fully implicit.

At each axial level a simultaneous solution for all subchannel enthalpies, densities, crossflows, axial flows and pressures is required before proceeding to the next. This is done in two separate stages which require first an iterative solution of the energy equation (3.13), followed by another iterative solution of the combined momentum equations (3.14) and (3.15). The following subsection provides the details of the formation of the implicit enthalpy solution. The derivation of the flow solution will follow.

3.1.2 Implicit Energy Equation

The fluid energy equation is solved simultaneously with the conducting wall energy equation. From Section 4, the wall energy balance is expressed by

$$\frac{1}{\Delta t} [(\rho c L \Delta Y)]_j \{T_w - T_w^n\}_j + \{D_w^T\} [LH] [D_w] \left\{ \begin{matrix} T \\ T_w \end{matrix} \right\}_j = 0 \quad (3.19)$$

Equations (3.18) and (3.19) are solved for subchannel enthalpies and wall temperatures by converting the subchannel temperatures to enthalpies as follows.

The temperatures in the transverse coolant conduction term are converted via the transformation

$$\{D_c^T\} \left[\frac{CS\bar{K}}{L_c} \right] [D_c] \{T_j\} = \{D_c^T\} [C_c] [D_c] \{h_j\}$$

where the coefficient C_c is a diagonal matrix defined as

$$[C_c] = \left[\frac{CS\bar{K}}{L_c} \right] [D_c] \{\hat{T}_j\}_D [D_c] \{\hat{h}_j\}_D^{-1}$$

and the operator $\{[X]\}_D$ is the diagonal matrix $[\zeta]$ such that $\zeta_{n,n} =$ the nth term of the vector $\{X\}$.

The coolant temperatures in the wall heat transfer equations are transformed using a difference definition of specific heat of the form

$$c_p = \frac{h_j - \hat{h}_j}{T_j - \hat{T}_j} \text{ or } T_j = \frac{h_j}{c_p} + (\hat{T}_j - \frac{\hat{h}_j}{c_p}). \text{ Substituting these}$$

definitions for T_j in Equations (3.16) and (3.19) produces

$$\begin{aligned} & \frac{1}{\Delta t} A_j \left(\rho_j^{n-h} f_g \frac{\partial \psi}{\partial h} \right) \hat{h}_j + \frac{m_{j-1} \hat{h}}{\Delta X} h_j + \{D_C^T\} \{\hat{h} * \tilde{w}_j\} - \hat{h}_j \{D_C^T\} \{\tilde{w}_j\} + \\ & \{D_C^T\} [w' + C_C] [D_C] \{\hat{h}_j\} - \{D_W^T\} [LH] [D_W] \left\{ \begin{matrix} h/c_p \\ T_w \end{matrix} \right\}_j = \\ & \frac{1}{\Delta t} \bar{A}_j \left(\rho_j^{n-h} f_g \frac{\partial \psi}{\partial h} \right) \hat{h}_j^n + \frac{m_{j-1} \hat{h}}{\Delta X} h_{j-1} + \{D_R^T\} [P \phi \bar{H}] [D_R] \left\{ \begin{matrix} \hat{T} \\ T_R \end{matrix} \right\}_j + \\ & \frac{1}{\Delta X^2} \left(k A_j (\hat{T}_{j+1} - \hat{T}_j) - k A_{j-1} (\hat{T}_j - \hat{T}_{j-1}) \right) - \\ & \{D_W^T\} [LH] [D_W] \left\{ \begin{matrix} \hat{T} - \hat{h}/c_p \\ 0 \end{matrix} \right\}_j \end{aligned} \quad (3.20)$$

$$\begin{aligned} & \frac{1}{\Delta t} (\rho c \Delta Y) T_{wj} + \{D_W^T\} [LH] [D_W] \left\{ \begin{matrix} h/c_p \\ T_w \end{matrix} \right\}_j = \\ & \frac{1}{\Delta t} (\rho c \Delta Y) T_{wj}^n - \{D_W^T\} [LH] [D_W] \left\{ \begin{matrix} \hat{T} - \hat{h}/c_p \\ 0 \end{matrix} \right\}_j \end{aligned} \quad (3.21)$$

Equations (3.20) and (3.21) are combined to produce a set of NC + NW equations from which the coolant enthalpies and wall temperature are calculated. This set has the form

$$\begin{bmatrix} C_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{Bmatrix} \hat{h} \\ T_w \end{Bmatrix}_j + \begin{bmatrix} 0 & 0 \\ 0 & C_2 \end{bmatrix} \begin{Bmatrix} \hat{h} \\ T_w \end{Bmatrix}_j + [D_W]^T [LH] [D_W] \begin{Bmatrix} \hat{h} \\ T_w \end{Bmatrix}_j = \begin{Bmatrix} B_1 \\ B_2 \end{Bmatrix} \quad (3.22)$$

where

$[C_1]$ is an NC x NC matrix containing the coefficients in the first five terms of Equation (3.20)

$[C_2]$ is an NW x NW array containing the coefficient in the first term of Equation (3.21)

$\{B_1\}$ is the vector of length NC which contains all terms to the right of the equal sign in Equation (3.20) and

$\{B_2\}$ is the vector of length NW which contains the terms to the right of the equal sign in Equation (3.21).

The composite matrices of Equation (3.22) are combined to form an (NC + NW) set of equations which have the form

$$[AAH] \begin{Bmatrix} h_j \\ T_{wj} \end{Bmatrix} = \{BH\}$$

This form is solved by an iterative procedure for the unknown coolant enthalpy and wall temperature distributions.

3.1.3 Momentum Equations

The two momentum equations (3.17) and (3.18) are combined to form an expression that is solved for the crossflow at j in terms of the lateral pressure difference and axial flows at the $j-1$ position. The new axial flows at j can then be found from the new crossflows via continuity.

The m_j terms are eliminated from the momentum equation (3.17), by direct substitution of the finite difference continuity equation (3.15). The irrecoverable pressure loss term dependency on m_j is reduced using the identity $m_j^2 = m_{j-1}^2 + (m_j - m_{j-1})(m_j + m_{j-1})$, which is approximated in the solution scheme by using continuity again for $m_j - m_{j-1}$ as

$$m_j^2 = m_{j-1}^2 + \Delta X \left(\frac{\rho_j - \rho_j^n}{\Delta t} + \{D_C^T\} \{w_j\} \right) 2\bar{m}$$

Substituting the above for m_j^2 in Equation (3.17) and rearranging produces the form of the axial momentum equation which can be combined with the lateral momentum equation (3.18):

$$\begin{aligned}
 p_j = p_{j-1} + \Delta X \left\{ - \left(K_L + \frac{(\hat{v}/A)_j - (\hat{v}/A)_{j-1}}{\bar{A}\Delta X} \right) \frac{m_{j-1}^2}{g_c} - \rho \cos \theta - \right. \\
 \left. \{D_c^T\} \{w'\} [D_c] \{u_j\} + \frac{\rho_j - \rho_j^n}{g_c \Delta t} \left[\frac{\Delta X}{\Delta t} + (\hat{v}/A)_j + K_L \bar{A} \Delta X \right] 2\bar{m} \right\} + \\
 \frac{1}{\bar{A}g_c} \frac{m_j^n - m_{j-1}}{\Delta t} \left\{ + \left[\left(\frac{\Delta X}{\Delta t} \{D_c^T\} - \{D_c^T\} \{u_j^*\} \right) \frac{1}{\bar{A}} + \right. \right. \\
 \left. \left. \frac{1}{\bar{A}} \left((\hat{v}/A)_j + K_L \bar{A} \Delta X \right) 2\bar{m} \{D_c^T\} \right] \{w_j\} \right\}
 \end{aligned} \tag{3.23}$$

Equations (3.23) and (3.18) are combined to form a system of NK equations that is solved for the unknown crossflows.

Equation (3.23) is written as

$$\{p_{j-1}\} = \{p_j\} - \{F\}\Delta X - [R_j]\{w_j\}\Delta X \tag{3.24}$$

where F_j consists of the terms multiplied by ΔX and R_j contains coefficients of $\{W\}$ in Equation (3.23).

Equation (3.18) is rearranged and written as

$$[D_c]\{p_{j-1}\} = [RP]\{w\} + \{FP\} \tag{3.25}$$

where

$$[RP] = \left[\frac{1}{\left(\frac{S}{l}\right)} \frac{1}{\Delta t} + \frac{\{u_j^*\}}{\Delta X} + \{C_j\} \right] \tag{3.26}$$

$$\{FP\} = \frac{S}{\ell} \frac{C_S}{S^2} [D_C] [D_C^T] \left\{ (N) \cos \Delta\beta \frac{\tilde{w}_j^2}{\rho} \right\} - \frac{S}{\ell} \frac{\{w_j^n\}}{\Delta t} + \frac{\{u^*w\}_{j-1}}{\Delta X} \quad (3.27)$$

Applying the $[D_C]$ operator to Equation (3.24), the pressure difference between subchannels at elevation $j-1$ is

$$[D_C]\{p_{j-1}\} = [D_C]\{p_j\} - [D_C]\{F\}\Delta X - [D_C][R_j]\{w_j\}\Delta X \quad (3.28)$$

Combining Equation (3.28) with (3.25) produces a set of simultaneous equations which is solved for the lateral flow distribution w at each axial location:

$$[AAA]\{w_j\} = \{b_j\} \quad (3.29)$$

where

$$[AAA] = [D_C][R_j]\Delta X + [RP] \quad (3.30)$$

and

$$\{b_j\} = [D_C]\{p_j - F\Delta X\} - \{FP\} \quad (3.31)$$

3.1.4 Solution Procedure

The overall solution scheme consists of an external iterative sweep of the computational mesh from inlet to exit in which local values of h , ρ , w , m and p are updated at each axial level in turn. This involves two additional internal iterative solutions for the enthalpies in all subchannels and the crossflows in all gaps at each level. The external solution is considered to be converged when the maximum change in crossflow, axial flow and enthalpy is simultaneously

less than the specified input value between successive external iterations. If the convergence criteria are not satisfied after a specified number of external iterations, the calculation is terminated. Convergence criteria and maximum iterations are similarly specified for the two internal iterative solutions but the solution is allowed to continue whether or not these are satisfied.

The boundary conditions for the flow solution are a specified inlet flow and enthalpy distribution, zero inlet crossflow and uniform pressure (zero lateral pressure difference) at the exit. A uniform overall pressure drop may be specified instead of the inlet flow, as will be discussed later. Since the subchannels are connected only to each other, no additional lateral boundary condition is needed. The fuel rod and conducting wall models to be described in Section 4 supply a thermal boundary condition for the energy equation.

In the steady state, the initial estimates of h , w , and m required to begin the iteration at axial position j are defined as the values resulting from the solution at $j-1$ and $j+2$ and the specified inlet boundary values when $j=1$. The subchannel pressures are calculated after the fact. Only the pressure difference between subchannels is required during the iteration and its initial estimate is defined as $[D_c] \{p_j\} = 0$. In transients, the initial values of the variables are those computed in the previous time step.

The overall solution sequence is illustrated in flow-chart form in Figure 3-2. Before each external channel sweep, the fuel rod model is solved over the entire mesh using surface heat transfer coefficients and subchannel temperatures from the preceding iteration. Before the first iteration, these quantities are not available so the fuel model is

FIGURE 3-2. Implicit Solution Sequence

bypassed and the input value of heat flux is supplied directly to the energy equation. After the first external iteration, the fuel model supplies fuel surface temperatures that are used with the surface heat transfer coefficient to calculate the energy input to the fluid.

The first operation at each axial level in the external channel sweep is the iterative solution of the combined subchannel and wall energy equation (3.22) for all subchannel enthalpies and wall temperatures. The updated enthalpies provide new subchannel densities via the equation of state; these are used in evaluating the coefficients and source terms of the combined momentum equation (3.29). Also at this time new heat transfer coefficients are calculated for use in the fuel model before the next external iteration. The crossflows which result from the iterative solution of Equation (3.29) are used in the continuity equation (3.15) with the new densities and the axial flows at the preceding level to compute the new axial flows. This completes the update of the flow field at axial level j . Before proceeding to the next level, the modified axial momentum equation (3.28) is solved using the new crossflows to provide a new estimate of the pressure difference between the subchannels at level $j-1$, $[D_c]\{p\}_{j-1}$. This step acts to propagate flow disturbances upstream because this change in $[D_c]\{p\}_{j-1}$ will cause a corresponding change to $[D_c]\{p\}_{j-2}$ in the next external iteration, and so on.

After all axial levels have been updated, the convergence criteria are checked to determine if another external iteration is needed. If not, the solution is printed out, and boundary conditions and forcing functions for a new time step are computed if applicable. If another iteration is

necessary, and the inlet flow is specified, the solution proceeds directly to the fuel model and the external channel sweep sequence is repeated. If the overall pressure drop is the boundary condition, the inlet flows are adjusted after each iteration to force the calculated pressure drop toward the desired value.

The expression for adjusting the inlet flow rate is based on the assumption that the total steady-state pressure drop, Δp_t , minus the gravitational head, Δp_g , is proportional to the square of the inlet flow rate, m_1 :

$$\Delta p \equiv \Delta p_t - \Delta p_g = C m_1^2 \quad (3.32)$$

where C is a proportionality constant. Given the desired value for the total pressure drop, Δp_{bc} , the flow adjustment required is approximated by

$$m_1 - \tilde{m}_1 = \frac{dm_1}{d\Delta p} (\Delta p_{bc} - \tilde{\Delta p}_t) \quad (3.33)$$

where the tilde superscript denotes the value from the last external iteration. The derivative is determined directly from Equation (3.32) as

$$\frac{dm_1}{d\Delta p} = \frac{1}{2C m_1} \quad (3.34)$$

Assuming small changes in C and Equation (3.34),

$$C = \frac{\Delta p}{m_1^2} \sim \frac{\tilde{\Delta p}}{\tilde{m}_1^2} \quad (3.35)$$

and, therefore

$$\frac{dm_1}{d\Delta p} = \frac{\tilde{m}_1}{2\tilde{\Delta p}} \quad (3.36)$$

Substituting Equation (3.36) into (3.33), the flow adjustment becomes

$$m_1 = \tilde{m}_1 \left(1 + \frac{\Delta p_{bc} - \tilde{\Delta p}_t}{2(\tilde{\lambda}_{p_t} - \tilde{\lambda}_{p_g})} \right) \quad (3.37)$$

Because the solution is iterative and an error in the denominator does not affect the solution at convergence, the subchannel gravitational head, $\tilde{\lambda}_{p_g}$, is estimated using the mean of the average inlet and outlet densities:

$$\tilde{\lambda}_{p_g} = \beta Z \cos \theta (\bar{\rho}_{inlet} + \bar{\rho}_{exit}) \quad (3.38)$$

where Z is the total channel length, θ is the angle from vertical and β is a damping factor (usually 0.8). In addition, the total pressure drop in the denominator of Equation (3.37) is taken as the average pressure drop over all subchannels:

$$\Delta \bar{p}_t \equiv \frac{\sum_{i=1}^{N_C} A_i \tilde{\Delta p}_i}{\sum_{i=1}^{N_C} A_i} \quad (3.39)$$

where A is the subchannel area.

The final expression for flow adjustment is formed by combining Equations (3.38) and (3.39) with (3.37).

$$m_1 = \tilde{m}_1 \left(1 + \frac{\Delta p_{bc} - \tilde{\Delta p}_t}{2\Delta \bar{p}_t - \beta Z \cos \theta (\bar{\rho}_{inlet} + \bar{\rho}_{exit})} \right) \quad (3.40)$$

3.2 EXPLICIT METHOD

The procedure in most finite difference solutions of partial differential equations is to set up a spatial computational mesh to represent the desired physical configuration.

The computational variables are then assigned positions on the mesh points, and the partial differential equations are simulated by forming differences of the main variables across specified mesh points to represent the derivatives.

The philosophy used in deriving the finite differences in equations for the COBRA explicit solution differs somewhat. Instead of performing the solution by simulating partial differential equations, the cell balance equations from which the partial differential equations are derived are solved directly. In this way it is much easier to keep track of the discrete nature of the subchannel and the physical meaning of the variables. Although the end result is essentially the same, this approach can make it easier to avoid many of the pitfalls of finite differences and to keep the solution as "physical" as possible.

To solve the cell balance equations, some assumptions must be made about the nature of the two-phase flow field to relate the area and volume averaged quantities. In the explicit solution, two-phase flow is currently assumed to be completely homogeneous with the phases in thermal equilibrium. The homogeneous assumption implies that the phase velocities are equal and the phase distribution is uniform throughout the control volumes. The equilibrium assumption requires the phases to be at the same pressure and temperature.

The use of these assumptions reduces the area average mass flux to a function of vapor volume fraction and velocity. The mass flux is defined as

$$\langle \rho u \rangle = \langle \alpha \rho_v u_v \rangle + \langle (1-\alpha) \rho_l u_l \rangle \quad (3.41)$$

where α is the vapor volume fraction and the subscripts, v and l , refer to the vapor and liquid phases, respectively. If ρ_v and ρ_l are constant and $u_v = u_l = u$ uniform throughout the control volume, then

$$\langle \rho u \rangle = u[\langle \alpha \rangle \rho_v + (1 - \langle \alpha \rangle) \rho_l] \quad (3.42)$$

Since α is also considered uniform in the control volume, the area and volume averages are equivalent so that

$$\langle \rho u \rangle = \langle \langle \rho \rangle \rangle u \quad (3.43)$$

By the same process, the enthalpy flux can be written as

$$\langle \rho h u \rangle = \langle \langle \rho h \rangle \rangle u \quad (3.44)$$

or, if the average enthalpy, h , is defined as

$$h \equiv \frac{\langle \langle \rho h \rangle \rangle}{\langle \langle \rho \rangle \rangle} \quad (3.45)$$

Equation (3.44) can be related to the mass flux by Equations (3.43) and (3.45) as

$$\langle \rho h u \rangle = h \langle \langle \rho \rangle \rangle u = h \langle \rho u \rangle \quad (3.46)$$

The average enthalpy is related to phase enthalpies by the static quality or vapor mass fraction, x , defined as

$$x \equiv \frac{\alpha \rho_v}{\langle \langle \rho \rangle \rangle} \quad (3.47)$$

from which

$$h = xh_v + (1-x)h_\ell \quad (3.48)$$

By repeating this process the entire set of balance equations is expressed in terms of $\langle \rho u \rangle$, $\langle \rho v \rangle$, $\langle \langle \rho \rangle \rangle$, h as defined above, and p . The mass fluxes are combined with the dimensions by defining

$$m \equiv \langle \rho u \rangle A \quad (3.49)$$

and

$$w \equiv \langle \rho v \rangle S \quad (3.50)$$

These five quantities--axial mass flow rate, m , lateral mass flow rate per unit axial length, w , mixture average density, ρ , static enthalpy, h , and pressure, p --are the primary variables in the explicit scheme. The definitions of these and several auxiliary variables are summarized in Table 3-1.

3.2.1 Difference Equations

To form the difference equations, computational cells of the same form as shown in Figure 3-3 are used. It is natural and convenient to define the state variables ρ , p and h at the center of the cell and the flux variables m and w on the axial and lateral surfaces, respectively, as shown in Figure 3-3. Each of the two momentum equations, then, uses a separate control volume centered around the respective flow. The offset momentum cells place each flow rate directly between the two pressures that are the dominant terms in the momentum

FIGURE 3-3. Placement of Primary Variables on a Computational Cell

forcing function. Also, the density and enthalpy are centered between all the flows necessary for their computation in the continuity and energy equations.

The major variables are indexed by axial level as shown in Figure 3-3. Auxiliary indexes required to identify specific gaps and channels have been omitted for clarity.

Where two or more variables appear in sequence with only one subscript, all are assumed to have that subscript. Thus, $\rho h_j = \rho_j h_j$. All terms on the right-hand sides of the following equations are computed from previous time step information and the dependent variables on the left sides are unknowns. Using the index convention with the variables positioned as shown, the cell balance equations for mass, energy, axial momentum and lateral momentum are rewritten as:

Mass

$$\hat{A}_j \Delta X \frac{\partial}{\partial t} \rho_j + m_j - m_{j-1} + \Delta X \{D_C^T\} \{w_j\} = 0 \quad (3.51)$$

Energy

$$\begin{aligned} \hat{A}_j \Delta X \frac{\partial}{\partial t} \rho h_j + m h_j^* - m h_{j-1}^* + \Delta X \{D_C^T\} \{w h_j^*\} = \\ \Delta X \{D_r^T\} [P \Phi H] [D_r] \{T_j\} + \Delta X \{D_w^T\} [LH] [D_w] \{T_j\} + \\ \frac{1}{\Delta X} \left[\hat{A} k_j (T_{j+1} - T_j) - \hat{A} k_{j-1} (T_j - T_{j-1}) \right] - \\ \Delta X \{D_C^T\} \left[CS \frac{\bar{k}}{L_C} \right] [D_C] \{T_j\} - \Delta X \{D_C^T\} [w'] [D_C] \{h_j\} \end{aligned} \quad (3.52)$$

Axial Momentum

$$\begin{aligned} \frac{\partial}{\partial t} m_j + \hat{A}_j \frac{1}{\Delta X} (p_{j+1} - p_j) + 1/2 \left(\frac{f}{D_h} + \frac{K}{\Delta X} \right) \left(\frac{m^2}{\rho^* A} \right)_j - \\ \frac{1}{\Delta X} (\hat{u} m_{j+1}^* - \hat{u} m_j^*) - \{D_C^T\} \left\{ S \hat{v} \left(\frac{m}{A} \right)_j^* \right\} = -\hat{A} \hat{\rho}_j \cos \theta - \\ F_T \{D_C^T\} [\hat{w}'] [D_C] \{u_j'\} \end{aligned} \quad (3.53)$$

Lateral Momentum

$$\begin{aligned} \frac{\partial}{\partial t} w_j - \frac{S}{\ell} \{D_C\} \{p_j\} - \frac{1}{\Delta X} (\bar{u} w_j^* - \bar{u} w_{j-1}^*) - \\ \{D_C\} [D_C^T] \{ (N) (wv)_j \cos \Delta \beta \} = -1/2 K_{GL} \frac{S}{\ell} |v| w_j - S \bar{\rho}_j \sin \theta \cos \theta \end{aligned} \quad (3.54)$$

The donor cell method has been uniformly employed to compute the convected quantities. That is, the enthalpy convected by m_j in the energy equation is denoted by h^* and is defined as

$$\begin{aligned} h_j^* &= h_j \text{ if } m_j > 0 \\ h_j^* &= h_{j+1} \text{ if } m_j < 0. \end{aligned} \quad (3.55)$$

In crossflow convection, the convected variable is selected from one of the adjacent channels based on the sign of the crossflow. The enthalpy carried by w_j in the energy equation is defined as

$$h_j^* = h_k \text{ if } w_j > 0$$

$$h_j^* = h_l \text{ if } w_j < 0 \quad (3.56)$$

where k and l are adjacent channel indices and the positive direction for crossflow is from k to l . In the momentum equations, where some averaging is required to define the convecting velocities, the donor cell selection is made before the averaging is performed. This process is illustrated in Table 3-2 which shows how each of these quantities is computed.

The donor cell method is "physical", easy to compute and enhances computational stability at the expense of high numerical diffusion which tends to "smear out" sharp gradients across the computation mesh. Methods are available to reduce this effect but they either produce additional disturbances which can be more detrimental than the diffusion, demand excessive additional computation time or storage, or are not applicable to multidimensional problems. For these reasons, numerical diffusion is tolerated in most problems.

A notable exception is vertical two-phase flow at low speeds where gravity provides a physical means to keep density gradients sharp. An artificial liquid/vapor equal volume exchange rate is optionally computed at cell boundaries based on the amount of liquid and vapor in neighboring cells. This exchange produces a net flow of liquid downward until the lower cell is completely liquid or the upper cell is completely vapor. This net flow is incorporated only in the mass and energy conservation equations;

**TABLE 3-2. Computation of Averages
and Donor Cell Products**

Term	Definition	Usage
$\hat{A}_j$	$1/2(A_j + A_{j-1})$	Continuity and Energy
$\hat{\hat{A}}_j$	$1/2(\hat{A}_j + \hat{A}_{j+1})$	Axial Momentum
mh_j^*	$\begin{cases} m_j h_j, & m_j > 0 \\ m_j h_{j+1}, & m_j < 0 \end{cases}$	Axial Energy Transport
wh_j^*	$\begin{cases} w_j h_k, & w_j > 0 \\ w_j h_\ell, & w_j < 0 \end{cases}^{(a)}$	Lateral Energy Transport
$\hat{k}_j$	$1/2(k_{j+1} + k_j)$	Thermal Conductivity for Axial Conduction
$\bar{k}_j$	$1/2(K_k + K_\ell)_j$	Thermal Conductivity for Lateral Conduction
u_j	$\begin{cases} (m/A)_j^{1/\rho_j}, & m_{j+1/2} > 0 \\ (m/A)_j^{1/\rho_{j+1}}, & m_{j+1/2} < 0 \end{cases}$	Axial velocity
$\hat{u}_j$	$1/2(u_j + u_{j-1})$	Axial Momentum Transport Velocity
$\hat{u}m_j$	$\begin{cases} \hat{u}_j m_{j-1}, & \hat{u}_j > 0 \\ \hat{u}_j m_j, & \hat{u}_j < 0 \end{cases}$	Axial Momentum Transport in Axial Direction
v_j	$\begin{cases} (w/S)_j^{1/\rho_k}, & w_j > 0 \\ (w/S)_j^{1/\rho_\ell}, & w_j < 0 \end{cases}$	Lateral Velocity
$S\hat{v}(m^*/A)_j$	$1/2[Sv_{j+1}(m^*/A)_j + Sv_j(m^*/A)_j]^{(b)}$	Axial Momentum Transport in Lateral Direction
$Sv_j(m^*/A)_j$	$\begin{cases} Sv_j(m_k/A_k)_j, & v_j > 0 \\ Sv_j(m_\ell/A_\ell)_j, & v_j < 0 \end{cases}$	
$\hat{w}'_j$	$1/2(w'_j + w'_{j+1})$	Turbulent Crossflow
$\bar{u}_j$	$1/2(u_k + u_\ell)_j$	Average Axial Velocity in a Gap
$\bar{u}w_j^*$	$1/2[u_k w^{*+} + u_\ell w^{*-}]_j^{(c)}$	Axial Transport of Lateral Momentum
$u_\ell w^*$	$\begin{cases} u_\ell w_j, & u_\ell > 0 \\ u_\ell w_{j+1}, & u_\ell < 0 \end{cases}$	
$\bar{\rho}_j$	$1/2(\rho_k + \rho_\ell)$	Average Density in a Gap
$\hat{\rho}$	$1/2(\rho_j + \rho_{j+1})$	

(a) The k and ℓ indices refer to adjacent channels. Positive direction for crossflow is from k to ℓ .

(b) Terms are similarly defined. Both use $(m_k/A_k)_j$ and $(m_\ell/A_\ell)_j$. See next line.

(c) Terms are similarly defined. Both use w_j and w_{j+1} . See next line.

there are no explicit momentum effects. Given some maximum exchange velocity, V , the total rate mass addition, S_j , to a cell, j , by this process is computed by

$$S_j = V(\rho_f - \rho_g) [A_j(1 - \alpha_{j+1})\alpha_j - A_{j-1}(1 - \alpha_j)\alpha_{j-1}] \quad (3.57)$$

The exchange velocity, V , is an input constant in COBRA-IV.

3.2.2 The ACE Method

The basis for the explicit solution is the ACE method (Advanced Continuous-fluid, Eulerian) developed at PNL to calculate the motion of fluid with steep density gradients approaching liquid-vapor interface conditions (Stewart and Rowe, 1976). The method is an extension of the basic ICE technique (Harlow and Amsden, 1971) as modified over the past several years. In the conventional application of ICE and its successors, an explicit energy equation using flows and energies from the previous time step to form the convective terms is employed. In many low speed two-phase flow applications, these explicit convective terms can lead to severe computational difficulty where steep density gradients exist. The ACE method eliminates this problem by making the energy convective terms implicit and combining the energy equation directly with continuity and the state relation.

To illustrate the method, consider the following abbreviated forms of Equations 3.51 through 3.54.

Mass

$$\hat{A}_j \Delta X (\rho_j - \rho_j^n) + m_j - m_{j-1} + \Delta X \{D_C^T\} \{w_j\} = 0 \quad (3.58)$$

Energy

$$\hat{A}_j \frac{\Delta X}{\Delta t} (\rho h_j - \rho h_j^n) + m h_j^* - m h_{j-1}^* + \Delta X \{D_c^T\} \{w h_j^*\} = Q_j^n \quad (3.59)$$

Axial Momentum

$$m_j = m_j^n - \Delta t \frac{\hat{A}_j}{\Delta X} (p_{j+1} - p_j) - \Delta t F_j^n \quad (3.60)$$

Lateral Momentum

$$w_j = w_j^n + \Delta t \frac{S}{\ell} \{D_c\} \{p_j\} - \Delta t G_j^n \quad (3.61)$$

All explicit terms have been combined into the variables Q^n , F^n and G^n , respectively. All other variables not specifically superscripted n are assumed to be new time implicit values. In addition, the reference pressure equation of state is retained from the implicit solution in Section 3.1,

$$\rho = \rho(h, p^*) \quad (3.62)$$

By inverting the state equation, all the enthalpies in Equation (3.59) can be expressed in terms of the specific volume, v . For example,

$$h_j^* = h_o + \left. \frac{\partial h}{\partial v} \right|_p (v_j^* - v_o) \quad (3.63)$$

where h_o and v_o define some arbitrary reference state close enough to h^* and v^* so that $\partial h / \partial v$ can be assumed constant between the two states.

Applying Equation (3.63) to the energy equation (3.59) yields the following result:

$$mv_j^* - mv_{j-1}^* + \Delta X [D_C^T] \{wv_j^*\} - \frac{\partial v}{\partial h} \bigg|_p Q_j^n =$$

$$\left(v_o - \frac{\partial v}{\partial h} \bigg|_p h_o \right) \left[\hat{A}_j \frac{\Delta X}{\Delta t} (\rho_j - \rho_j^n) + m_j - m_{j-1} + \Delta X \{D_C^T\} \{w_j\} \right]$$

(3.64)

From continuity, the right-hand side of Equation (3.64) reduces to zero.

The left side of Equation (3.64) is the basis of the ACE method. It simply relates the divergence of the velocity field to the volumetric expansion caused by heat transfer. Since it deals with changes in volume rather than changes in mass, this divergence equation can easily consider the motion of the steepest density gradients. It is solved simultaneously with the momentum equations in an iterative procedure similar to that used by Hirt and Cook (1972). The pressures and flows are adjusted sequentially in each computational cell using a Newton-Raphson procedure to reduce the residual error in the divergence equation. The solution procedure is discussed in detail in the following section.

The solution scheme begins a time step by solving the fuel model and evaluating the explicit terms Q , F and G . Initial estimates for the flows, $\tilde{m}$ and $\tilde{w}$, are obtained from the momentum equations based on pressures and flows from the previous time step or initial conditions. These tentative flows will not generally satisfy Equation (3.64) but will yield a residual error, E_j . That is,

$$\tilde{mv}_j^* - \tilde{mv}_{j-1}^* + \Delta X \{D_C^T\} \{wv_j^*\} - \frac{\partial v}{\partial h} \bigg|_p Q_j^N = E_j \quad (3.65)$$

The objective is to reduce this residual error to zero in all computational cells. This is done by adjusting the pressures and flows in each cell sequentially in an iterative loop.

The pressure change, Δp_j , necessary to reduce E_j to zero in any computational cell is computed by using the total derivative of E with respect to pressure. That is,

$$\Delta p_j = \frac{-E_j}{dE/dp} \quad (3.66)$$

The total derivative is formed as follows, holding the specific volume constant:

$$\frac{dE}{dp_j} = \frac{\partial E}{\partial \tilde{m}_j} \frac{d\tilde{m}}{dp_j} + \frac{\partial E}{\partial \tilde{m}_{j-1}} \frac{d\tilde{m}_{j-1}}{dp_j} + \frac{\partial E}{\partial \tilde{w}_j} \frac{dw}{dp_j} \quad (3.67)$$

The momentum equations (3.60) and (3.61) provide linear relations for the flow differentials

$$\frac{d\tilde{m}_j}{dp_j} = \frac{\Delta t}{\Delta X} \hat{A}_j \quad (3.68)$$

$$\frac{d\tilde{m}_{j-1}}{dp_j} = -\frac{\Delta t}{\Delta X} \hat{A}_{j-1} \quad (3.69)$$

$$\frac{d\tilde{w}_j}{dp_j} = -\Delta t \frac{S}{\ell} \{D_c\} \frac{d\{p\}}{dp_j} \quad (3.70)$$

The partial derivatives of E with respect to the flows are found directly from Equation (3.65). The final result is

$$\frac{dE}{dp} = \frac{\Delta t}{\Delta X} \left[v^* \hat{A}_j + v^* \hat{A}_{j-1} + \Delta X \frac{S}{\ell} \{D_c^T\} [v_j^*] [D_c] \frac{d\{p\}}{dp_j} \right] \quad (3.71)$$

After the necessary pressure change is computed by Equation (3.66), the flows, density and enthalpy in the cell are updated. The new flows are found via the momentum derivatives, Equations (3.68) through (3.70). These flows are then used in the continuity equation (3.58) to find the new density (and specific volume). Finally, a new enthalpy is found from the equation of state using the new density and the reference pressure. This procedure is repeated over all computational cells until the maximum error, E , is less than some specified value. The solution is then considered to be converged and, after the normal bookkeeping chores, the calculations for the time step are complete. The above sequence is illustrated in Figure 3-4.

It is important that the density and enthalpy are continually updated inside the iteration and that no acceleration is used to attempt to speed the convergence. The pressure and flow changes calculated by Equation (3.66) for cell j guarantee satisfaction of continuity in that particular cell but will disturb the mass balance in neighboring cells. Although this disturbance becomes smaller as the iteration proceeds, a finite error remains at convergence and a new density calculated after iteration terminates will contain this residual error. Allowing this error to appear in the density may cause problems near saturation conditions. It can be eliminated from the density by computing the new density immediately after the pressure and flow adjustment in each cell. The small residual error then shows up as a small deviation in velocity, normally considerably less critical than density.

Acceleration is not used because it would modify the pressure change and introduce a continuity error. In practice,

FIGURE 3-4. Explicit Solution Sequence

acceleration has provided only a 20 percent saving in computation time at best. This is considered a small price to pay for the absence of significant extraneous density deviations.

Large hydraulic resistances are encountered in many applications. For example, a loss coefficient on the order of 10 is required to represent pressurized water reactor (PWR) inlet nozzles and associated hardware and a value of about 700 is required to model the resistance of the primary system from the upper plenum to the cold legs through the steam generator and pumps. The pressure drop, Δp_f , across a computational cell due to a loss coefficient of this type is normally calculated explicitly. For example,

$$\Delta p_f = K |u_j^n| m_j^n \quad (3.72)$$

It can be shown that a numerical stability criterion for an explicit momentum equation with explicit hydraulic resistance is

$$\Delta t < \frac{\Delta X}{(1+K) |u|} \quad (3.73)$$

where Δt is the maximum time step and K is the maximum loss coefficient considered. When a large value of K is used in combination with high velocities this limitation can clearly be prohibitive.

This severe time step restriction can be circumvented by treating the flow resistance semi-implicitly using new-time flows to compute the pressure drop. Equation (3.72) is rewritten as

$$\Delta p_f = K |u_j^n| m_j^{n+1}$$

The linearized definition for the pressure losses is applied to the momentum equations (3.60) and (3.61), resulting in the expressions

$$m_j = \left[m_j^n - \Delta t F_j - \hat{A}_j \frac{\Delta t}{\Delta X} (p_{j+1} - p_j) \right] \frac{1}{(1 + \Delta t K |u|_j)} \quad (3.74)$$

$$w_j = \left\{ w_j^n - \Delta t G_j + \frac{S}{\ell} \Delta t \{D_c\} \{p_j\} \right\} \frac{1}{(1 + \Delta t K_G |v|_j)} \quad (3.75)$$

When these new momentum pressure relations are used in calculating the pressure cell pressure correction, the total derivative of E with respect to p, Equation (3.71), takes the form

$$\begin{aligned} \frac{dE}{dp} = \frac{\Delta t}{\Delta X} & \left\{ \left(\frac{v^* \hat{A}}{1 + \Delta t K |u|} \right)_j + \left(\frac{v^* \hat{A}}{1 + \Delta t K |u|} \right)_{j-1} + \right. \\ & \left. \Delta X \frac{S}{\ell} \{D_c^T\} \left\{ \left(\frac{v^*}{1 + \Delta t K_G |v|} \right) \right\}_j \{D_c\} \right\} \end{aligned} \quad (3.76)$$

Other than substituting Equation (3.76) above for Equation (3.71) and modifying the flow pressure derivatives (3.60) through (3.70), the original solution procedure is not altered. This approach removes any stability limitations arising from the use of large hydraulic resistances.

3.3 NUMERICAL PERFORMANCE

Implicit and explicit hydrodynamic computation methods were presented in Sections 3.1 and 3.2. Both are very powerful analytical tools that can be applied to a great many problems but it must be remembered that they will never give mathematically exact solution and there are even conditions under which they give no solution at all! Assuming the input is correct and none of the derivational assumptions is violated, the foregoing solution methods remain finite difference approximations to differential equations which, in turn, only approximate reality. They are subject to various numerical errors which, at best, decay with each iteration or time step as fast as new errors appear, but, at worst, grow without bound and destroy the calculation. Because both methods use iterative solution procedures, there will always be some small error left after any finite number of iterations. Assuming stability, the amount of error left is a measure of the degree of convergence of the solution. Another error is caused by the necessity of representing the problem by a finite number of discrete space and time steps. Details finer than the mesh and events occurring within one time step are obscured.

For the very simplest finite difference equation systems, it is possible to quantify the effects of these phenomena mathematically. However, a complete mathematical error and stability analysis is currently impossible for a complex nonlinear code like COBRA. There is no way to compute the accuracy of the final solution beforehand. Instead, a degree of judgment must be employed, relying on previous measurements of the code's accuracy compared to analytical solutions or experimental data. Rigorous numerical stability analyses are also developed only for simple linear systems. Several necessary conditions can be developed mathematically but it is currently impossible to predict analytically that a particular calculation will reach a convergent stable solution with any certainty. In this case,

experience must be substituted for analysis. One develops intuitive criteria for which problems tend to be unstable or require excessive computation time and the conditions required for their successful solution.

The purpose of this section is to document this experience as quantitatively as possible so that COBRA may be applied more confidently by the user community. Two main areas will be discussed: transient stability criteria and iterative solution convergence.

3.3.1 Transient Stability

The various numerical stability criteria discussed in this section apply only to the explicit solution. The implicit method is unconditionally stable for all time steps. The time step restrictions derived here are summarized in Table 3-3.

TABLE 3-3. Summary of Explicit Time Step Restrictions

<u>Restriction</u>	<u>Source</u>	<u>Comment</u>
$\Delta t < \frac{\Delta X}{u + \frac{S\Delta X}{A} v}$	Momentum flux	Basis for time step adjustment in explicit scheme.
$\Delta t < \frac{cA\rho}{\Sigma U}$	Thermal coupling of fuel and fluid	ΣU is defined by Equation (3.83)
$\Delta t < \frac{\Delta X^2 \rho c}{2k}$	Fuel axial conduction	Use fuel properties

The procedure applied most often to develop stability criteria for COBRA-IV has been the "positivity rule" which states simply that the new value of a dependent variable in a computational cell must be proportional to its old value. If the cell density was high at the last time step, for example, it ought to be high at the new time even though it is increasing or decreasing. If this rule is violated, the calculation may be

unstable. To illustrate, consider an explicit finite difference equation for one-dimensional energy transport in incompressible flow:

$$\frac{1}{\Delta t}(h_j^{n+1} - h_j^n) + \frac{u}{\Delta X}(h_j^n - h_{j-1}^n) = 0 \quad (3.76)$$

Solving for h_j^{n+1} yields

$$h_j^{n+1} = h_j^n \left(1 - \frac{u\Delta t}{\Delta X}\right) + \frac{u\Delta t}{\Delta X} h_{j-1}^n \quad (3.77)$$

Now, for h_j^{n+1} to remain proportional to its old time value, h_j^n , the coefficient must remain positive. This requires that

$$\frac{u\Delta t}{\Delta X} < 1 \quad (3.78)$$

the familiar Courant condition for explicit advection. Because ΔX is fixed and u is usually a dependent variable, the time step, Δt , must be adjusted to satisfy Equation (3.78).

Applying the positivity rule to the axial and lateral momentum equations (3.53) and (3.54), the conditions are

$$\frac{1}{\Delta t} - \frac{u}{\Delta X} - \frac{Sv}{A} > 0 \quad (3.79)$$

and

$$\frac{1}{\Delta t} - \frac{u}{\Delta X} > 0 \quad (3.80)$$

The axial gravity term, axial and lateral drag terms and the lateral momentum flux are not included. From Equations (3.79) and (3.80), the most restrictive time step restriction is

$$\Delta t < \frac{\Delta X}{u + \frac{S \Delta X}{A} v} \quad (3.81)$$

Although the convective part of the energy equation (3.52) is implicit, a second time step limitation arises from its explicit coupling to the fuel model. That is, the surface heat transfer is computed from the fluid temperature at the last time step. The time step criterion is

$$\Delta t < \frac{C A \rho}{\sum U} \quad (3.82)$$

where C is the fluid specific heat and $\sum U$ is the sum of all heat conductances affecting the fluid cell. At most,

$$\begin{aligned} \sum U = & \left\{ D_R^T \right\} \left\{ P \Phi H \right\} + \left\{ D_w^T \right\} \left\{ L H \right\} \\ & + \left\{ D_C^T \right\} \left\{ C S \bar{K} \right\} + \frac{1}{\Delta X^2} \left\{ \hat{k} A_j + \hat{k} A_{j-1} \right\} \end{aligned} \quad (3.83)$$

This condition does not apply in two-phase flow because the fluid temperature is constant. This makes the specific heat, and therefore the maximum time step, infinite.

The maximum time step defined by Equation (3.81) will generally be the most severe restriction. The thermal time step limit, Equation (3.82), is important only for problems with small channels and very high heat transfer coefficients as in LMFBR bundles.

One additional potential stability problem occurs in the fuel model. It is caused by the explicit treatment of the axial conduction terms for both the cladding and the fuel material. This type of instability has never been observed in normal LMFBR or LWR fuel simulations at PNL, but it may prove important in special cases where the axial node length is very small. The associated time step restriction is expressed by

$$\Delta t < \frac{\Delta X^2 \rho c}{2k} \quad (3.84)$$

where c is the heat capacity and k is the thermal conductivity. The condition should be checked for both the fuel and clad properties.

Because almost any transient calculation of interest involves changing conditions, the time step initially selected to satisfy all the stability requirements may not be sufficient later on. On the other hand, if a very small time step is chosen to satisfy the most severe conditions expected, the problem may take many more steps than necessary. For maximum efficiency, the time step size must be adjusted each time step as the computation progresses.

Time step adjustment in COBRA is accomplished solely on the basis of Equation (3.81), the convective Courant condition. After the flow solution is complete, a new time step, Δt^{n+1} , is calculated by

$$\Delta t^{n+1} = 2 \left(\frac{1}{\Delta t'} + \frac{1}{\Delta t^n} \right)^{-1} \quad (3.85)$$

where Δt^n is the current time step and

$$\Delta t' = \frac{C \Delta X}{u + \frac{S \Delta X}{A} v} \quad (3.86)$$

The Courant number, C , and a maximum permissible value for $\Delta t'$ are input quantities. A good value for C is 0.2 and it should never be more than about 0.7. Actually, a tradeoff occurs between the number of time steps required and the number of iterations in each time step. In most cases, the potential time saving using a Courant number of 0.5 instead of 0.2, for example, is completely reversed because each time step now requires 100 iterations instead of 10. In many cases, much computer time can be saved by taking smaller time steps! The code is working most efficiently at about 10-15 iterations per time step.

Equation (3.86) would be sufficient to compute a new time step but it is put in parallel with the old time step to provide some damping and to force the selection of the smallest reasonable time step. Where very large and very sudden changes occur, such as initiation of low pressure boiling, the time step just cannot adjust fast enough and the calculation may fail. In these cases, it is often best to run the problem in a series of shorter transients using COBRA's restart feature. When a "sudden change" instability is observed, that section can be restarted with a smaller maximum time step to get over the transition.

3.3.2 Convergence

In numerical mathematics, convergence is the property of finite differences that reduce to differential equations when space and time increments approach zero in the limit. In conventional usage, however, convergence will refer to the achievement of a stable iterative solution to within some specified error criteria. Specifically the effect of relatively "tight" or "loose" convergence criteria and the price paid in computer time to satisfy them will be discussed. Since the implicit and explicit iterative solutions are structured differently, they will be discussed separately.

The explicit scheme requires the convergence of but one iterative procedure. This is the overall pressure, flow and density field solution. To reduce errors in the density, no acceleration or damping factors are used as was brought out in Section 3.2. The criterion for convergence is the ratio of the divergence error to the cell volume. That is, the solution is converged when

$$\max \left| \frac{E_j \Delta t}{\hat{A}_j \Delta X} \right| < \epsilon \quad (3.87)$$

Generally, the looser the convergence, the less computation time required. However, since the small amount of error left

over at convergence serves as a minor flow disturbance for the next time step, there is a point beyond which increasing ϵ requires more iterations and may even cause the solution to become unstable. A good value of ϵ for single-phase liquids is 10^{-4} to 10^{-5} . In two-phase situations, up to 0.005 is tolerable. An ϵ greater than 10^{-2} will probably produce unreliable results.

The implicit scheme uses three iterative solutions: the separate internal loops for enthalpy and crossflow and the external channel sweep. Each requires one or more convergence and acceleration/damping criteria. The external channel sweep is the most important level of iteration to consider because it is probably the most sensitive.

Two convergence criteria must be simultaneously satisfied in the external loop. The rate of change of crossflow and axial flow must both be less than a specified value. That is,

$$\left| \frac{\tilde{m} - m^r}{m} \right| < \epsilon_m \quad (3.88)$$

and

$$\left| \frac{\tilde{w} - w}{w_c} \right| < \epsilon_w \quad (3.89)$$

where ϵ_m and ϵ_w are input constants and m and w are the axial and transverse flow rates. The tilde superscript indicates the current iterate value and w_c is defined as

$$w_c = 0.001 (\bar{w}_j / w_{k,j})^2 + w_{k,j} \quad (3.90)$$

where

$$\bar{w}_j = \frac{1}{N_k} \sum_{k=1}^{N_k} w_{k,j}$$

This type of normalization was chosen because in many problems there are regions where relatively small crossflows exist. Since these small crossflows have little effect on enthalpy or flow rate distributions a tight convergence is not required. The normalizing factor forces the required convergence on relatively large crossflows but loosens the convergence requirement on the smaller crossflows to make the computation more efficient.

The effect of using this type of normalizing factor is illustrated in Table 3-4, giving the value of ϵ_w required to achieve the same degree of convergence that would result if the criterion were $\left| \frac{\bar{w} - w}{w} \right| \leq 0.01$.

TABLE 3-4. Equivalent Convergence Criteria

<u>w</u>	<u>$\bar{w}/w$</u>			
	<u>0.01</u>	<u>0.1</u>	<u>1.</u>	<u>10.</u>
0.0001	0.01	0.009	0.0009	0.000009
0.01	0.01	0.01	0.009	0.0009
1.	0.01	0.01	0.01	0.009

In using the COBRA-IV implicit scheme, many problems converge very rapidly to acceptable rates of change for enthalpy and axial flow rate but the crossflow solution converges very slowly. If the required result of the calculation for this type of problem is subchannel temperature, quality, flow rate, etc., it is recommended that the calculation be stopped after N iterations. The result should then be examined and the problem repeated with the solution being printed after N+5 iterations. If the change in the important variables is small in the region of interest, then the solution can be considered converged for practical purposes. The above procedure can be accomplished easily using the COBRA restart option.

Other problems appear to be converging within the first four or five iterations but then tend to diverge. This behavior can

sometimes be corrected by using flow and pressure damping factors. It is recommended that values of 0.6 to 0.8 and 0.8 be used for the flow and pressure damping factors, respectively, when a problem tends to diverge. These factors damp iterative oscillations in the iterative flow rate and subchannel transverse pressure difference in the following manner:

$$m' = \alpha_m \tilde{m} + (1 - \alpha_m) m$$

$$\Delta p' = \alpha_p \tilde{\Delta p} + (1 - \alpha_p) \Delta p$$

where m' and $\Delta p'$ are the final values for the flow and lateral pressure difference, respectively.

Convergence is affected by the input geometry. As a general rule it is desirable to maintain the ratio of subchannel area/ ΔX^2 between 0.1 and 10. It also helps to use a value of the S/ℓ (group 9) parameter, which is somewhat representative of the actual ratio of gap spacing to centroid-centroid distance. The ratio of areas of adjacent subchannels should also be in the range of $5 > A_i/A_j > 0.20$. If the area ratio falls outside this range, relatively small changes in the flow rate of the large channel produce a large change in flow rate of the smaller channel, which may result in a numerically unstable solution. Some problems, particularly those specifying a low flow rate with steep radial power gradients, are unstable using the implicit scheme and no amount of damping will produce a solution. However, these problems can be solved by using the explicit scheme.

The implicit solution scheme incorporates the solution of two sets of simultaneous equations internal to the channel sweep. The first set is solved for the radial enthalpy distribution and the second for the radial crossflow distribution. Both sets of equations are solved with a Gauss-Seidel iterative procedure. In using this procedure the solution is generally accelerated by applying an acceleration factor of the form

$$X' = \alpha \tilde{X} - (1 - \alpha)X \quad (3.91)$$

in which α is the acceleration factor and X is the unknown variable, either subchannel enthalpy or gap crossflow. For most problems, values in the range 1.2 to 1.6 will hasten the procedure. Because the enthalpy coefficient matrix is strongly diagonally dominant, the enthalpy acceleration factor is set to a value of 1.5. The crossflow acceleration factor, however, is an input variable which defaults to 1.6 if not specified. If the solution of the crossflow coefficient array requires less than the allowable number of internal iterations, changing the value of the crossflow acceleration factor has little effect on the stability of the solution. If, on the other hand, the crossflow solution consistently requires all of the allowed iterations, the solution may be stabilized by using a smaller crossflow acceleration factor.

The convergence limit on the internal iterations for crossflow is set loosely because tight convergence is not required until the external iteration approaches its solution. This is accomplished by defining the internal convergence limit in the crossflow as the maximum of either the specified convergence limit or the lesser of 0.01 or 0.01 times the maximum external error, i.e.

$$\epsilon_w' = \max \left\{ \epsilon_w, \min \left(0.01, 0.01 * \max \left\{ \frac{\tilde{w}_{k,j} - w_{k,j}}{w_{cj}} \right\} \right) \right\} \quad (3.92)$$

The convergence limit on the enthalpy in the energy equation is set internally to a rate of change and less than 10^{-6} . That is, $\left| \frac{\tilde{h} - h}{h} \right| < 10^{-6}$. It is necessary to converge tightly because errors from the internal solution tend to grow as the external solution sweeps through the channel. However, because the enthalpy coefficient array is strongly diagonally dominant, the solution is rapid and a tight convergence does not appreciably retard the solution.

4.0 CONDUCTIVE HEAT TRANSFER

The conductive heat transfer models in COBRA compute internal temperature distributions within heat conducting materials and the surface heat fluxes to adjacent fluid channels. The models are interfaced with the fluid thermal-hydraulic solution using surface heat transfer coefficients.

Two independent conduction models are available: a detailed cylindrical or plate fuel heat transfer model that computes internal temperatures and surfaces heat fluxes based on the volumetric heat generation rate, and a lumped parameter model that computes the heat transfer between coolant channels on opposite sides of a heat conducting wall. These models are used in both the implicit and explicit thermal hydraulic solution schemes described in Section 3.

4.1 FUEL MODEL

The fuel heat transfer model calculates the internal temperature distribution within a solid material and can include the effects of axial conduction and temperature-dependent fuel thermal conductivity considered.

The solution (Cena et al., 1975) is a combination of the Method of Weighted Residuals (MWR) in the radial coordinate and finite differences in time and the axial coordinate. In MWR, orthogonal collocation is employed to determine the form of an approximate polynomial solution (Finlayson, 1972). MWR affords a higher order of accuracy by using the roots of orthogonal polynomials as the nodal positions where the solution is evaluated. This method maintains the accuracy and computing time of conventional finite difference schemes while computer storage is reduced by a factor of two.

4.1.1 Fuel Interior

The heat conduction model in COBRA-IV is derived from the fundamental heat conduction equation

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q''' \quad (4.1)$$

where k is the local thermal conductivity and q''' is the volumetric rate of heat generation.

This equation is expanded in two dimensions for both planar and cylindrical geometry with the radial coordinate nondimensionalized using the relationship $r = r'/R$, where r' is the radial coordinate and R is the fuel radius:

$$\rho c \frac{\partial T}{\partial t} = \frac{1}{R^2 r^{a-1}} \frac{\partial}{\partial r} r^{a-1} k(T) \frac{\partial T}{\partial r} + \frac{\partial}{\partial X} k(T) \frac{\partial T}{\partial X} + q''' \quad (4.2)$$

$a = 1$ Planar

$a = 2$ Cylindrical

Equation (4.2) is reduced to a linear partial differential equation using Kirchoff's transformation:

$$\theta = \frac{1}{k_0} \int_{T_0}^T k(T) dT = G(T) \quad (4.3)$$

where k_0 is the conductivity at reference temperature T_0 .

Differentiating Equation (4.3) with respect to r and t yields

$$\frac{\partial \theta}{\partial r} = \frac{d\theta}{dT} \frac{\partial T}{\partial r} = \frac{k(T)}{k_0} \frac{\partial T}{\partial r} \quad (4.4)$$

and

$$\frac{\partial \theta}{\partial t} = \frac{d\theta}{dT} \frac{\partial T}{\partial t} = \frac{k(T)}{k_0} \frac{\partial T}{\partial t} \quad (4.5)$$

which, when substituted into the differential equation (4.2), yields the transformed equation

$$\rho c \frac{k_o}{k(T)} \frac{\partial \theta}{\partial t} = \frac{k_o}{R^2 r^{a-1}} \frac{\partial}{\partial r} r^{a-1} \frac{\partial \theta}{\partial r} + \frac{\partial}{\partial X} k(T) \frac{\partial T}{\partial X} + q'' \quad (4.6)$$

This equation is solved numerically by a combination of techniques.

In the present application the radial coordinate is approximated by a symmetric polynomial of the form

$$\theta(r) = d_1 + d_2 r^2 + d_3 r^4 + \dots + d_N r^{2N-2}$$

or

$$\theta(r) = \sum_{i=1}^N (r^{2i-2}) d_i \quad (4.7)$$

Evaluating this polynomial at the N radial positions gives

$$\theta(r_j) = \sum_{i=1}^N (r_j^{2i-2}) d_i \quad (4.8)$$

or, in matrix notation,

$$\{\theta\} = [Q]\{d\}$$

where

$$Q_{ji} = r_j^{2i-2}$$

In the orthogonal collocation method, the radial positions are taken to be the roots to orthogonal polynomials, which affords accuracy comparable to finite element techniques. The radial positions or collocation points defined by Finlayson (1974) for a second-order approximation (N=3) are shown in Figure 4-1.

FIGURE 4-1. Fuel Rod Noding Using Second-Order Orthogonal Collocation

From Equation (4.8) the first and second derivatives are evaluated:

$$\left. \frac{d\theta}{dr} \right|_{r_j} = \sum_{i=1}^N (2i-2) r_j^{2i-3} d_i \quad (4.9)$$

and

$$\frac{1}{r^{a-1}} \frac{\partial}{\partial r} r^{a-1} \frac{\partial \theta}{\partial r} = \sum_{i=1}^N (2i-2)(2i+a-4) d_i r^{2i-4} \quad (4.10)$$

which, when written in matrix notation with $\{d\}$ replaced by $[Q]^{-1}\{\theta\}$, gives:

$$\frac{d}{dr}\{\theta\} = [C][Q]^{-1}\{\theta\} \quad (4.11)$$

and

$$\frac{1}{r^{a-1}} \frac{\partial}{\partial r} r^{a-1} \frac{\partial}{\partial r} \{\theta\} = [D][Q]^{-1} \{\theta\} \quad (4.12)$$

where

$$C_{ji} = (2i-2)r_j^{2i-3}$$

$$D_{ji} = (2i-2)(2i+a-4)r_j^{2i-4}$$

Substituting Equation (4.12) for the second derivative in Equation (4.6) yields

$$\rho c \frac{k_o}{k(T)} \frac{\partial \theta}{\partial t} = \frac{k_o}{R^2} [B] \{\theta\} + \frac{\partial}{\partial X} k(T) \frac{\partial T}{\partial X} + q''' \quad (4.13)$$

where

$$[B] = [D][Q]^{-1}$$

The axial conduction term is calculated by a central finite difference and the time derivative is approximated by a forward finite difference. Substituting these difference forms into Equation (4.13) yields the heat conduction model solved at N-1 interior nodal positions:

$$\frac{\rho c k_o}{\Delta t k_i} \theta - \frac{k_o}{R^2} \sum_{\ell=1}^N B_{i\ell} \theta_{\ell} = \frac{\rho c k_o}{\Delta t k_i} \theta_i^n + q''' + \frac{2}{\Delta X^2} \left[\frac{T_{j-1}^n - T_i^n}{\frac{1}{k_{j-1}} + \frac{1}{k_i}} + \frac{T_{j+1}^n - T_i^n}{\frac{1}{k_{j+1}} + \frac{1}{k_i}} \right] \quad (4.14)$$

where the superscript, n, denotes previous time, j - 1 and j + 1 denote adjacent axial levels at radial position i and k_i is k(T) at radial position i. The calculation of the second axial derivative as represented by the last term in Equation (4.14) is spatially explicit. That is, the required temperatures are taken

from the previous iteration. When used in the explicit hydraulic solution, these temperatures are also temporally explicit with the temperatures taken from the previous time step. Thus the tilde superscript indicates previous iteration when used with the implicit hydraulic solution, and previous time step (equivalent to "n" superscript) when used with the explicit hydraulic solution.

4.1.2 Fuel-Clad Interface

The boundary condition at the fuel surface is handled by a lumped resistance technique similar to that used in COBRA-IIIC. The governing equation is

$$-\frac{k_o}{R} \frac{\partial \theta}{\partial r} = H_g (T_N - T_{N+1}) \quad (4.15)$$

where N and N + 1 denote the fuel and clad exterior surfaces, respectively. The term H_g is defined by

$$\frac{1}{H_g} = \frac{1}{H_c} + \frac{Y_c}{k_c}$$

where Y_c and k_c are the cladding thickness and conductivity and H_c is the fuel-clad gap conductance.

Applying orthogonal collocation, Equation (4.11) is substituted for the first derivative in Equation (4.15), yielding

$$-\frac{K_o}{R} \sum_{\ell=1}^N A_{N\ell} \theta_{\ell} = H_g (T_N - T_{N+1}) \quad (4.16)$$

where $[A] = [C] [Q]^{-1}$ from Equation (4.11).

4.1.3 Cladding

A transient energy balance for the lumped clad is

$$\rho c \frac{\partial T_{N+1}}{\partial t} = \frac{H_g}{Y_c} \left(\frac{r_N}{r_{N+1}} \right)^{a-1} (T_N - T_{N+1}) - \frac{H_s}{Y_c} (T_{N+1} - \tilde{T}_f) + k_c \frac{\partial^2 \tilde{T}_{N+1}}{\partial X^2} \quad (4.17)$$

where H_s is the clad surface heat transfer coefficient and T_f is the fluid temperature.

Equation (4.17) is transformed using Kirchoff's transformation with an implicit time derivative and an explicit axial conduction term. The resulting equation is

$$\frac{(\rho c)_c}{\Delta t} \frac{k_o}{k_{N+1}} \theta_{N+1} = \frac{(\rho c)_c}{\Delta t} \frac{k_o}{k_i} \theta_{N+1}^n + \frac{k_c}{\Delta X^2} (\tilde{T}_{\ell+1} - 2\tilde{T}_{N+1} + \tilde{T}_{\ell-1}) + \frac{H_g}{Y_c} \left(\frac{r_N}{r_{N+1}} \right)^{a-1} (T_N - T_{N+1}) - \frac{H_s}{Y_c} (T_{N+1} - \tilde{T}_f) \quad (4.18)$$

To evaluate the implicit temperatures T_N and T_{N+1} in Equations (4.16) and (4.18), a truncated Taylor series is used:

$$T = T^n - \frac{G(T^n) - \theta(T^n)}{G'(T^n)} \quad (4.19)$$

where the function G is defined in Equation (4.3) and G' is the derivative of G with respect to T .

4.1.4 Solution Procedure

The boundary equations (4.16) and (4.18) are combined with the differential equation (4.14) to yield the matrix equation of the form

$$[a]\{\theta\} = \{Q\} \quad (4.20)$$

for the transformed temperatures at one axial level. This equation is solved by an iterative Gauss-Siedel procedure. The matrix elements of Equation (4.20) are shown in Figure 4-2.

Once the $\{\theta\}$ solution vector is determined, the temperature solution is evaluated using Equation (4.19) with $\theta(T^n)$ specified. If any elements of $[a]$ or $\{Q\}$ are temperature-dependent, the procedure is repeated until the resulting temperature change remains within a set limit and the solution is considered converged.

This sequence is repeated at each axial level to the ends of the fuel with additional axial sweeps if axial conduction is being considered. Normally, axial conduction has little effect and only two or three additional iterations are necessary. The resulting temperature solution supplies the surface heat flux for the fluid energy equation (3.16).

4.2 WALL MODEL

The heat transfer between fluid channels separated by a heat conducting wall is computed using a lumped parameter, single-cell heat conduction model. As with the more detailed fuel conduction model, the wall model is used in both flow solutions but the methods are different. With the implicit flow solution, the wall energy balance is solved simultaneously with the fluid energy equation to provide fully implicit coupling. The explicit scheme solves the wall energy balance independently to compute a heat flux that is applied explicitly to the fluid energy equation. The form of the wall equation remains the same in both cases.

The wall lies between two adjacent channels, i and j , along their full length and is described in terms of a thickness, Y_w , and length, L_w , with a constant, uniform heat capacity, $(\rho c)_w$,

$$[A] = \begin{bmatrix} \frac{\rho c R^2}{\Delta t k_1} - B_{11} & -B_{12} & -B_{13} & 0 \\ -B_{21} & \frac{\rho c R^2}{\Delta t k_2} - B_{22} & -B_{23} & 0 \\ A_{31} & A_{32} & A_{33} + \frac{H_g R}{k_o G_3'} & -\frac{H_g R}{k_o G_4'} \\ 0 & 0 & -\frac{H_g D}{Y_c G_3'} & \frac{(\rho c)_c k_o}{\Delta t k_5} + \frac{DH_g + H_s}{Y_c G_4'} \end{bmatrix}$$

$$\text{where } D \equiv \left(\frac{r_N}{r_{N+1}} \right)^{a-1}$$

$$\{Q\} = \left\{ \begin{aligned} & \frac{\rho c R^2}{\Delta t k_1} \theta_1^n + \frac{q_1 R^2}{k_o} + \frac{2R^2}{k_o \Delta X^2} \left[U_1^- (T_{\ell-1} - T_1) + U_1^+ (T_{\ell+1} - T_1) \right] \\ & \frac{\rho c R^2}{\Delta t k_2} \theta_2^n + \frac{q_2 R^2}{k_o} + \frac{2R^2}{k_o \Delta X^2} \left[U_2^- (T_{\ell-1} - T_2) + U_2^+ (T_{\ell+1} - T_2) \right] \\ & \frac{H_g R}{k_o} \left(T_4 - T_3 + \frac{G_3}{G_3'} - \frac{G_4}{G_4'} \right) \\ & \frac{(\rho c)_c k_o}{\Delta t k_4} \theta_4 + \frac{H_g D}{Y_c} \left(T_3 - T_4 + \frac{G_4}{G_4'} - \frac{G_3}{G_3'} \right) + \frac{H_s}{Y_c} \left(T_f - T_4 + \frac{G_4}{G_4'} \right) \\ & \quad + \frac{Y_c}{\Delta X^2} (T_{\ell+1} - 2T_4 + T_{\ell-1}) \end{aligned} \right\}$$

$$\text{where } \frac{1}{U_1^+} \equiv \frac{1}{k_{\ell+1}} + \frac{1}{k_i} \quad \frac{1}{U_1^-} \equiv \frac{1}{k_{\ell-1}} + \frac{1}{k_i}$$

FIGURE 4-2. Fuel Conduction Matrix Elements

as shown in Figure 4-3. The heat conductance, U , to each channel is defined in terms of a surface coefficient, H , and a conduction component, K_w/Y as

$$\frac{1}{U_i} = \frac{1}{H_i} + \frac{Y_i}{k_w} \quad (4.21)$$

In terms of these definitions, the wall energy balance is written in finite difference form as

$$\frac{(\rho c)_w Y_w}{\Delta t} (T_w - T_w^n) + U_i (T_w - T_i) + U_j (T_w - T_j) = 0 \quad (4.22)$$

where the n superscript refers to the past time step. Equation (4.22) is rearranged and rewritten in terms of the wall-channel connection matrix, $\{D_w\}$ described in Section 2 to yield

FIGURE 4-3. Conducting Wall Model Layout

$$\left(\frac{(\rho c)_{wLwYw}}{\Delta t} \right) T_w + \{D_w^T\} [L_w U] [D_w] \begin{Bmatrix} T \\ T_w \end{Bmatrix} = \left(\frac{(\rho c)_{wLwYw}}{\Delta t} \right) T_w^n \quad (4.23)$$

where $\begin{Bmatrix} T \\ T_w \end{Bmatrix}$ indicates the combined vector of subchannel and wall temperatures. Equation (4.23) is solved simultaneously with the fluid energy equation (3.16) in the implicit scheme. In the explicit solution, the fluid temperatures are taken from the previous time step and Equation (4.23) becomes

$$\begin{aligned} & \left(\frac{(\rho c)_{wLwYw}}{\Delta t} \right) T_w + \{D_w^T\} [L_w U] [D_w] \begin{Bmatrix} O \\ T_w \end{Bmatrix} = \\ & \left(\frac{(\rho c)_{wLwYw}}{\Delta t} \right) T_w^n - \{D_w^T\} [L_w U] [D_w] \begin{Bmatrix} T^n \\ O \end{Bmatrix} \end{aligned} \quad (4.24)$$

The corresponding heat flux, $\{Q\}$, to the fluid channels is then computed from the new wall temperatures by

$$\{Q\} = [D_w^T] [L_w U] [D_w] \begin{Bmatrix} T^n \\ T_w \end{Bmatrix} \quad (4.25)$$

5.0 CONSTITUTIVE RELATIONS

Throughout the development of the COBRA code a consistent effort has been made to keep the code as general as possible. As a result, it is possible in many cases to specify all necessary constitutive relations entirely with input data. The assumptions are made throughout that any correlation can be applied locally and to transients as well as the steady state. These assumptions must be carefully evaluated in light of each specific application, especially when the user desires to insert other models into the code.

No assertion is made that the correlations presented in this section are the best in all cases. However, it should be emphasized that the character of the final solution often depends more strongly on the form of the governing equations than on the accuracy of the constitutive relations. The numerical phenomena associated with the finite difference approximations to the governing equations can have an equally powerful influence. Thus the physical, mathematical and computational aspects of the modeling process cannot be studied separately.

The preceding sections of this report have illustrated the derivation and solution of a set of five conservation equations: continuity, fluid energy, axial momentum, lateral momentum and heat conduction. These five equations plus a fluid state relation are sufficient to solve for the six dependent variables of fluid density and enthalpy, axial flow rate, lateral flow rate, pressure and fuel temperature. It is necessary, however, to supply specifications for the surface heat transfer coefficient,

friction factor, phase slip ratio and turbulent mixing parameter to close the set for a complete solution. The formation of these four constitutive relations and the equation of state will be discussed in this section.

5.1 FLUID STATE RELATION

The main purpose of the equation of state in COBRA is to provide a relation between fluid density and enthalpy. Other temperature-dependent properties such as thermal conductivity and viscosity must also be related to the enthalpy. Since the code is applicable to liquids, gases and two-phase mixtures, no single function or correlation can cover the entire range. Therefore, a separate procedure is used for each of the three states. Subcooled liquid properties are assumed to follow the saturation line and are input in tabular form. In the two-phase region, density and enthalpy are related by various void-quality functions while the rest of the properties remain at the saturated liquid value. Superheated steam properties are available in COBRA in the form of a table which is internally calculated from steam table correlations for specific reference pressures. Properties for other gases and vapors at a constant pressure can also be input as liquid properties. Linear interpolation is used in all cases to calculate values between table entries.

All fluid property calculations in COBRA use the concept of a reference pressure which is uniformly applied over the entire computational mesh. The reference pressure is specified by input and may be made a function of time. It determines the saturation properties and is the pressure at which the superheated steam property table is set up. By

using this concept, the fluid density is unaffected by the local momentum pressure or hydrostatic head. This makes fluid property calculation extremely fast and efficient on the computer but neglects compressibility effects. This approach is justifiable whenever the maximum spatial pressure change is small compared to the reference pressure, or when properties can be assumed independent of pressure as for a subcooled liquid.

5.1.1 Subcooled and Saturated Liquid Properties

A typical example of the liquid property table is shown in Table 5-1. The input variables are, from left to right, saturation pressure and temperature, liquid and vapor specific volume, liquid and vapor enthalpy, saturated liquid viscosity, thermal conductivity and surface tension. The pressure is used only to fix the saturation state; the temperature is used mainly for heat transfer. If the fluid is subcooled, the liquid specific volume and enthalpy determine the state and the vapor values are not used. In the two-phase region, both liquid and vapor specific volume and enthalpy are required to calculate void fraction and quality. The viscosity and conductivity are used to form the Reynolds and Prandtl numbers for use in other correlations; the conductivity is also used in fluid heat conduction calculations. For two-phase conditions, these two properties retain their saturation values. The surface tension is used only in an optional subcooled void model.

As an example of how Table 5-1 is used in the code, consider a single channel, heated uniformly such that boiling occurs near the exit. The inlet temperature will be 100°F with the system pressure 25 psia. At the inlet,

TABLE 5-1. Typical Water Property Table

P (Psi)	T (F)	VF (ft ³ /lb)	VG (ft ³ /lb)	HF (Btu/lbm)	HG (Btu/lbm)	VISC. (lb/hr-ft)	KF (Btu/hr-ft-F)	SIGMA (lb/ft)
.2	50.00	.01602	1704.80000	18.05	1083.40	3.15000	.33600	-0.00000
.3	60.00	.01603	1207.60000	28.06	1087.70	2.68000	.34200	-0.00000
.4	70.00	.01605	868.40000	33.05	1092.10	2.32000	.34600	-0.00000
.5	80.00	.01607	633.30000	48.04	1096.40	2.05000	.35300	-0.00000
.7	90.00	.01610	468.10000	58.02	1100.30	1.85100	.35800	-0.00000
A .9	100.00	.01613	350.40000	68.00	1105.10	1.64300	.36200	-0.00000
1.7	120.00	.01620	230.30000	87.97	1113.60	1.32100	.37000	-0.00000
2.9	140.00	.01629	123.00000	107.95	1122.00	1.11000	.37800	-0.00000
4.7	160.00	.01640	77.29000	127.96	1130.20	.94900	.38300	-0.00000
7.5	180.00	.01651	50.22000	148.00	1138.20	.77000	.38800	-0.00000
11.5	200.00	.01664	33.64000	168.08	1146.00	.7200	.39100	-0.00000
B 25.0	240.00	.01693	16.32000	208.45	1160.60	.57900	.39600	-0.00000
50.0	281.00	.01727	8.51400	250.20	1174.10	.49100	.39590	.00301
100.0	327.80	.01774	4.43100	298.50	1187.20	.41000	.39360	.00261
150.0	358.40	.01809	3.01390	330.60	1194.10	.36900	.38930	.00235
200.0	381.80	.01869	2.28730	355.50	1198.30	.34500	.38520	.00209
250.0	401.00	.01865	1.84320	376.10	1201.10	.32600	.38060	.00193
300.0	417.40	.01889	1.54270	394.00	1202.90	.31300	.37600	.00180
350.00	431.70	.01912	1.32550	409.80	1204.00	.30100	.37180	.00168
400.0	444.60	.01934	1.16100	424.20	1204.60	.29000	.36820	.00158
680.0	499.90	.02043	.67581	487.70	1202.30	.25500	.34940	.00117
920.0	534.60	.02130	.48901	530.00	1195.70	.23700	.33250	.00092
1080.0	554.00	.02188	.40902	554.60	1189.90	.22700	.32240	.00079
1280.0	575.40	.02262	.33603	582.90	1181.20	.21700	.30860	.00065
1440.0	590.80	.02323	.29156	604.00	1173.30	.21100	.29840	.00054
1680.0	611.50	.02420	.23978	634.00	1159.80	.20300	.28200	.00041
1920.0	630.00	.02526	.19978	662.70	1144.20	.19500	.26600	.00031
2160.0	646.80	.02647	.16752	690.80	1125.60	.18600	.24900	.00022
2320.0	657.20	.02739	.14916	709.50	1111.40	.17900	.23700	.00017
2480.0	666.90	.02845	.13266	729.10	1095.50	.17200	.22400	.00013

the code enters the table at 100°F--state A on Table 5-1--and assigns the fluid a specific volume of 0.01613 ft³/lb-in. and an enthalpy of 68.0 Btu/lb-in. with a corresponding viscosity and conductivity. Since the fluid enthalpy is below the saturation value of 208.45 Btu/lb-in. as defined by the 25 psia reference pressure--state B on Table 5-1--the vapor specific volume and enthalpy are ignored.

As the fluid is heated on its way up the channel, this process is repeated in each computational cell, employing linear interpolation where necessary, to determine the fluid specific volume and other properties in terms of the increasing enthalpy. When the enthalpy passes the saturation value of 208.45 Btu/lb-in. the code must find the specific volume in terms of quality so the saturated vapor quantities are required. Viscosity and conductivity would remain at 0.579 lb-in./hr-ft and 0.396 Btu/hr-ft-°F, respectively. If the enthalpy were to surpass the vapor enthalpy of 1160.0 Btu/lb, an error would occur unless superheated steam properties were used. Table entries with pressures higher than the reference pressure are ignored.

5.1.2 Two-Phase Properties

In the two-phase region as defined by the reference pressure and Table 5-1, the fluid density is related to the enthalpy in terms of a void fraction-quality relation. The simplest and probably most widely used is the homogeneous model in which the void fraction, α , is related to the equilibrium quality, x , by

$$\alpha = \frac{xv_g}{(1-x)v_f + xv_g} \quad (5.1)$$

where v_g and v_f are the vapor and liquid specific volumes, respectively. The quality is defined in terms of the mixture enthalpy by

$$x \equiv \frac{h-h_f}{h_g-h_f} \quad (0 \leq x < 1) \quad (5.2)$$

where h_g and h_f are the vapor and liquid enthalpies.

The explicit hydraulic solution derived in Section 3.2 uses only the homogeneous model. In the implicit solution, Section 3.1, three additional void-quality relations are available.

The first is a simple slip model that uses an input constant slip ratio, k . The homogeneous expression, Equation (5.1), is modified to yield

$$\alpha = \frac{xv_g}{(1-x)v_f k + xv_g} \quad (5.3)$$

where x is defined as before.

A modified Armand (1946) model is also available where

$$\alpha = \frac{(0.833+0.167x)xv_g}{(1-x)v_f + xv_g} \quad (5.4)$$

Finally, up to seven coefficients, a_i , may be specified for sixth-order polynomial function of the form

$$\alpha = a_0 + a_1x + a_2x^2 + \dots + a_nx^n \quad (n \leq 6) \quad (5.5)$$

As an alternative to the equilibrium quality definition, Equation (5.2), the Levy (1966) subcooled void model is available for the implicit solution only. This model calculates the true quality, x_t , in terms of the equilibrium quality, x ,

from Equation (5.2) and the quality at which bubble departure begins, x_d , by the expression

$$x_t = x - x_d e^{(x/x_d - 1)} \quad (x_d < x) \quad (5.6)$$

where x_d is defined by

$$x_d = \frac{c_p \Delta T}{(h_g - h_f)} \quad (5.7)$$

and ΔT is a function of the surface heat flux, friction factor, mass flux, and surface tension.

5.1.3 Superheated Steam Properties

If the fluid enthalpy exceeds the saturated vapor enthalpy from Table 5-1 at the reference pressure, the calculation is normally terminated. If water is being used, however, superheated steam properties are available in a precalculated table. Properties are calculated at the reference pressure from saturation temperature to a maximum temperature specified by input. If the reference pressure is changed by more than 0.1 percent in a transient problem, the steam property table is recalculated.

A typical example of a superheated steam property table is shown in Table 5-2. The properties are, from left to right, temperature, enthalpy, specific heat, specific volume, viscosity, thermal conductivity, and Prandtl number. Enthalpy and specific volume are evaluated with the relationships used in the Keenan and Keys (1936) steam tables and the specific heat is evaluated as $\Delta h / \Delta T$. Agreement with the ASME Steam Tables (Meyer et al., 1967) is within 1 percent for enthalpy and specific volume, and within 4 percent for the specific heat.

TABLE 5-2. Typical Superheated Steam Property Table

T (F)	M (Btu/lbm)	CP (Btu/lbm-ft)	V (ft ³ /lbm)	VISC. (lbm/ft-hr)	K (Btu/hr-ft-°F)	PR
290.4	1176.5	.553	7.1477	.0330	.0170	1.08
305.3	1184.5	.540	7.3197	.0339	.0172	1.06
320.2	1192.6	.529	7.4885	.0347	.0176	1.05
335.2	1200.5	.514	7.6549	.0356	.0179	1.02
380.0	1223.5	.500	8.1428	.0381	.0191	1.00
424.8	1245.9	.493	8.6190	.0407	.0204	.98
469.6	1268.0	.490	9.0875	.0432	.0218	.97
514.4	1290.0	.488	9.5509	.0457	.0233	.96
559.2	1311.8	.489	10.0106	.0482	.0248	.95
604.0	1333.7	.490	10.4676	.0507	.0264	.94
648.8	1355.7	.492	10.9226	.0533	.0280	.94
693.6	1377.7	.494	11.3759	.0558	.0297	.93
738.4	1399.8	.497	11.8281	.0582	.0314	.92
783.4	1422.1	.500	12.2792	.0606	.0331	.92
828.0	1444.5	.503	12.7296	.0631	.0349	.91
872.8	1467.0	.506	13.1793	.0655	.0367	.91
917.6	1489.7	.510	13.6284	.0680	.0385	.90
962.4	1512.5	.514	14.0771	.0704	.0404	.90
1007.2	1535.6	.517	14.5254	.0729	.0422	.89
1052.0	1558.7	.521	14.9733	.0753	.0441	.89
1096.8	1582.1	.525	15.4210	.0778	.0461	.89
1141.6	1605.6	.529	15.8684	.0802	.0480	.88
1186.4	1629.3	.533	16.3156	.0827	.0500	.88
1231.2	1653.2	.537	16.7626	.0851	.0519	.88
1276.0	1677.2	.541	17.2094	.0876	.0539	.88
1320.8	1701.5	.545	17.6561	.0900	.0559	.88
1365.6	1725.9	.549	18.1026	.0925	.0579	.88
1410.4	1750.5	.553	18.5491	.0949	.0599	.88
1455.2	1775.3	.558	18.9954	.0974	.0619	.88
1500.0	1800.3	.538	19.4416	.0998	.0639	.87

The viscosity and thermal conductivity are calculated by the equations listed in the 1967 ASME Tables where applicable. In regions not covered by these relationships, the recommended data interpolation given by McClintock and Silvestri (1968) is used. The equations are also extended in use from the recommended temperature limit of 1292°F to 1500°F. Agreement with tabular values in the 1967 ASME Tables is within ±6 percent.

5.2 HEAT TRANSFER CORRELATIONS

Surface heat transfer coefficients are required to couple the two hydraulic solutions to the fuel and wall models. In single-phase flows, the surface coefficient is also used in determining the start of nucleate boiling and in computing the hot wall viscosity correction. In the latter uses, the surface coefficient is computed directly from local subchannel conditions and is applied only to the heated perimeter of that channel.

In computing surface heat transfer from fuel rods, an average surface coefficient and an average fluid temperature around the rod is calculated from local subchannel variables. If ϕ_i is the input fraction of the rod perimeter facing channel i , the average temperature, $\bar{T}$, and surface coefficient, $\bar{H}$, for the rod are computed from the N subchannels around the rod by

$$\begin{aligned}\bar{T} &= \frac{1}{\bar{\phi}} \sum_{i=1}^N (\phi_i T_i) \\ \bar{H} &= \frac{1}{\bar{\phi}} \sum_{i=1}^N (\phi_i H_i)\end{aligned}\tag{5.8}$$

where $\bar{\phi} = \sum_{i=1}^N \phi_i$ and T_i and H_i are individual channel temperature and surface coefficients, respectively.

After new fuel temperatures are computed with the fuel model, the linear heat rate, q_i , to each channel from the fuel rod is computed by

$$q_i = \phi_i \pi D \bar{H} (T_r - \bar{T}) \quad (5.9)$$

where T_r is the rod surface temperature. This method conserves the energy transferred between rods and channels but it also contains the implicit assumptions of uniform fluid conditions around the rod and infinite circumferential heat conduction. As long as all $H_i \sim \bar{H}$ and $T_i \sim \bar{T}$ these assumptions are appropriate. However, if subchannel conditions are markedly nonuniform, the heat flux distribution will be incorrect.

This situation can be corrected quite easily by input at the expense of some increased computer storage and running time. The procedure is to specify a separate fuel rod for each fraction of the original rod exposed to a different subchannel. This forces the average fluid temperature and surface coefficient to equal the subchannel values by definition and also supplies a separate fuel surface temperature to each channel. This effectively assumes zero rod circumferential heat conduction. The effects of this change are illustrated in Figure 5-1, in which rod 1 is replaced by three equivalent rods, 1a, 1b and 1c for each of the three surrounding channels. Note that the three rods each must have exactly the same power, dimensions and material properties as the original rod.

FIGURE 5-1. Input Change for Zero Circumferential Conduction

5.2.1 Single-Phase Flow

Single-phase heat transfer includes both single-phase liquid and superheated steam flows. The surface coefficient, H , is computed as a function of the Reynolds and Prandtl numbers by

$$H = \frac{k_f}{D_h} \left(a \text{Re}^b \text{Pr}^c + d \right) \quad (5.10)$$

where k_f is the fluid conductivity, D_h is the channel hydraulic diameter and the constants a through d are either input or default to form the Dittus-Boelter correlation.

In addition to its main use with the fuel model, Equation (5.10) is also used to compute an average wall temperature difference, ΔT_w , by the expression

$$\Delta T_w = \frac{q'}{HP_h} \quad (5.11)$$

where q' is the total linear heat rate to the channel and P_h is its heated perimeter. This temperature difference is used in performing the hot wall viscosity correction and in the

Jens-Lottes correlation (Tong, 1972) defining the start of nucleate boiling.

5.2.2 Two-Phase Flow

In past versions of COBRA, the specification of two-phase heat transfer coefficients was left completely to the user because of the wide range of possible conditions the code might be called upon to consider. This is still much the case, but since many important applications involve boiling in water, the correlations and selection logic from the RELAP4 computer program (Moore and Rettig, 1973) are now available as an option.

Seven regimes are considered: forced convection, sub-cooled and nucleate boiling, forced convection vaporization, transition boiling, transition pool boiling, film boiling, and pool film boiling. Figure 5-2 shows the relative regions of applicability for each on a heat flux versus temperature plot. The correlations used for each regime are listed in Table 5-3. In addition to these correlations, a minimum heat transfer coefficient of $5 \text{ Btu/hr-ft}^2\text{-}^\circ\text{F}$ is assumed.

Three critical heat flux (CHF) correlations are used. The correlations and criteria for selection are shown in Table 5-3. Additionally, a minimum value of $90,000 \text{ Btu/hr-ft}^2$, the presumed value for a stagnant fluid, is assumed. When the mass flux is less than $2 \times 10^5 \text{ lb/hr-ft}^2$, the critical heat flux is interpolated between $90,000 \text{ Btu/hr-ft}^2$ and the value calculated via the appropriate correlation at a mass flux of $2 \times 10^5 \text{ lb/hr-ft}^2$.

The selection of the appropriate heat transfer correlation is based on three conditions. The first is an evaluation of the physical state. For example, if the clad temperature is below the saturation temperature, the forced convection regime

FIGURE 5-2. Region of Application of Heat Transfer Correlations

is appropriate. The second is the evaluation of the critical heat flux and the clad temperature that would exist at this heat flux. Comparison determines whether pre-CHF or post-CHF correlations are appropriate. The third criterion is the comparison of two or more calculated heat transfer coefficients in order to select the proper coefficient in regions where correlations overlap.

It should be understood that these correlations and associated logic were put together specifically for a system blowdown situation and thus should be applied very carefully. It has been found, for instance, that this package cannot be used in a low pressure reflooding configuration. In such cases, the user must modify the code to install alternate logic and correlations.

5.2.3 Critical Heat Flux Correlations

In the preceding section, critical heat flux correlations were used to define the boiling curve for computing the heat transfer coefficient. In this section their use in

TABLE 5-3. Heat Transfer and Critical
Heat Flux Correlations

HEAT TRANSFER CORRELATIONS

PRE-CHF

forced convection - Equation (5.10)

subcooled and nucleate boiling - Thom et al. (1966)

forced convection vaporization - Schrock and Grossman (1959)

POST-CHF

transition boiling - McDonough, Milich and King (1958)

stable film boiling - Groeneveld (1968)

low pressure film boiling - Dougall and Rohsenow (1963)

pool film boiling - Berenson (1961)

transition pool boiling - Moore and Rettig (1973)

forced convection to superheated vapor - Equation (5.10)

CRITICAL HEAT FLUX CORRELATIONS

1. $P/\text{psia} < 725$
Modified Barnett - Hughes (1970)
2. $725 < P/\text{psia} < 1000$
interpolation between Barnett (1966) and modified Barnett
3. $1000 < P/\text{psia} < 1300$
Barnett (1966)
4. $1300 < P/\text{psia} < 1500$
interpolation between Barnett (1966) and Babcock & Wilcox-2
- Gallerstedt et al. (1966)
5. $P/\text{psia} > 1500$
Babcock & Wilcox-2

the analysis of Departure from Nucleate Boiling (DNB) will be discussed. This feature of COBRA is entirely post-calculated from a completed thermal-hydraulic solution and does not affect the results in any way.

The characteristic parameter in DNB analysis is the Departure from Nucleate Boiling Ratio (DNBR), the ratio of the critical heat flux as calculated from local fluid conditions by an appropriate correlation to the actual heat flux at that location. Critical heat flux should occur at a DNBR of 1.0. DNBRs greater than 1.0 indicate that CHF has not yet occurred and the minimum DNBR, if greater than 1.0, provides a measure of the thermal margin of the channel.

In COBRA the critical heat flux is predicted with either the Babcock & Wilcox B&W-2 (Gellerstedt et al., 1966) or Westinghouse W-3 (Tong, 1965) CHF correlations using local fluid conditions from either the implicit or explicit thermal-hydraulic solutions. This predicted CHF is divided by the actual heat flux used in COBRA to compute a DNBR at each axial location in each channel. This data is then scanned for the minimum DNBR and the results are reported in a critical heat flux summary.

For a nonuniform axial heat flux distribution, Tong's (1972) shape factor is applied to both CHF correlations. At axial position X_j , the shape factor, F , is expressed as

$$F = \frac{C}{q'(X_j) (1 - e^{-C(X_j - X_{j0})})} \int_{X_0}^{X_j} q''(X) e^{-C(X_j - X)} dX \quad (5.12)$$

where C is a constant. In COBRA the integral is calculated as a summation of finite integrals, each taken over the calculation increment ΔX . Assuming a constant value of the heat flux $q''(X)$ over the interval, the integral from

X - ΔX to X is

$$q'(X) \int_{X-\Delta X}^X e^{-C(X_j-X)} dX = \frac{q''(X)}{C} e^{-CX_j} [e^{CX} - e^{C(X-\Delta X)}] \quad (5.13)$$

The entire integral in Equation (5.12) taken as a summation over the increments of ΔX from X_{j0} to X_j is

$$F = \frac{e^{-CX_j} \sum_{j=j_0+1}^J q''(X_j) (e^{CX_j} - e^{CX_{j-1}})}{q''(X_j) [1 - e^{-C(X_j - X_{j0})}]} \quad (5.14)$$

where $X_{j0} = 0$ is the axial location of the start of integration. For B&W-2, it is the channel inlet and for W-3 it is the start of local boiling defined by the Jens-Lottes correlation (Tong, 1972).

The corrected value of CHF is computed from the CHF calculated for a uniform heat flux and the shape factor by

$$q_{NU} = q_U / F \quad (5.15)$$

5.3 FRICTION FACTOR AND LOSS COEFFICIENTS

The friction factor is used to compute the axial pressure gradient from wall shear stress. The frictional pressure drop across one axial increment, ΔX, is computed by the expression

$$\Delta p_f = \frac{f \Delta X}{D_h} \frac{G^2}{2g\rho} \quad (5.16)$$

where D_h is the channel hydraulic diameter, G is the axial mass flux and ρ is the fluid density.

Local axial drag forces from flow obstructions such as grid spacers are accounted for by a local loss coefficient, K . The pressure drop across the obstruction is determined by

$$\Delta p_K = K \frac{G^2}{2g\rho} \quad (5.17)$$

Because of the complex geometry in a gap, a lateral frictional drag is not computed separately. Instead, the friction is lumped with form drag in a constant lateral loss coefficient, K_G . The lateral pressure drop, $\{D_c\}\{p\}$, across the gap is computed by

$$\{D_c\}\{p\} = K_G \frac{w^2}{2g\rho^* S^2} \quad (5.18)$$

where w is the crossflow per unit length, ρ^* is the density of the donor channel and S is the gap width. In rod bundle geometry, the value of K_G is typically 0.5.

5.3.1 Single-Phase Flow

For single-phase flows, Equations (5.16), (5.17) and (5.18) apply directly. The friction factor for Equation (5.16) is normally determined from the Reynolds number by

$$f = a \text{Re}^b + c \quad (5.19)$$

where a , b and c are input constants. If an additional expression is desired for laminar flows, another set of constants, ℓ , m , n , can be read in for a laminar friction factor, f_ℓ , defined by

$$f_\ell = \ell \text{Re}^m + n \quad (5.20)$$

When f_ℓ is computed, the friction factor for Equation (5.16) is taken as the maximum of f and f_ℓ from Equations (5.19) and (5.20).

Since the choice of input constants may be influenced by subchannel roughness and pitch-to diameter ratio, the code can accept up to four sets of constants that correspond to four subchannel types which may be assigned to the input subchannels.

The friction factor may also be corrected for heated wall viscosity by using Tong's (1968) relationship

$$f/f_o = 1 + \frac{P_h}{P_w} \left[\left(\frac{\mu_w}{\mu_b} \right)^{0.6} - 1 \right] \quad (5.21)$$

where f_o is the isothermal friction factor, P_h and P_w are the heated and wetted perimeters, respectively, and μ_w is the viscosity evaluated at the walls fluid temperature. The wall viscosity, μ_w , is evaluated at the temperature T_w , defined by

$$T_w = T_{bulk} + \Delta T_w \quad (5.22)$$

where ΔT_w is determined by Equation (5.11) from the average heat flux.

5.3.2 Two-Phase Flow

For two-phase flows, Equation (5.16) is rewritten to include a two-phase friction multiplier, ϕ ,

$$\Delta p_f = \frac{f\phi\Delta X G^2}{2D_h g \rho_f} \quad (5.23)$$

The multiplier currently may be specified by three different models: the homogeneous model, the Armand (1946) model, or as a polynomial function of quality. The homogeneous model

serves only to replace the liquid density in the denominator of Equation (5.23) with the mixture density, ρ , and is computed as a simple density ratio

$$\phi = \rho_f / \rho \quad (5.24)$$

The Armand model defines ϕ as a function of quality and void fraction in the following series of expressions.

$$\begin{aligned} \phi &= (1-x)/(1-\alpha)^{1.42} & 0.39 < (1-\alpha) \leq 1.0 \\ \phi &= 0.478 (1-x)^2/(1-\alpha)^{2.2} & 0.1 < (1-\alpha) \leq 0.39 \\ \phi &= 1.73 (1-x)^2/(1-\alpha)^{1.64} & 0 < (1-\alpha) \leq 0.1 \end{aligned} \quad (5.25)$$

The polynomial option is formed by up to seven input coefficients, a , used to express ϕ as a function of quality in the form

$$\phi = a_0 + a_1x + a_2x^2 + \dots + a_Nx^N \quad N \leq 6 \quad (5.26)$$

Only the homogeneous model is available in the explicit scheme and serves as the default for the implicit solution. The use of mixture density in the lumped drag force computations in Equations (5.17) and (5.18) has the same effect as a homogeneous friction multiplier.

5.4 TURBULENT MIXING

The model used for lateral turbulent energy and momentum exchange is based on a fluctuating equal mass exchange between

adjacent channels. This is expressed as a fluctuating cross-flow per unit length, w' , which is assumed to be proportional to the gap width, s , and the average axial mass flux, $\bar{G}$,

$$w' = \beta s \bar{G} \quad (5.27)$$

where

$$\bar{G} = \frac{G_i A_i + G_j A_j}{A_i + A_j} \quad (5.28)$$

for two adjacent channels of area, A_i and A_j . The proportionality constant, β , is the so-called mixing factor that must be specified by input or by correlation.

The turbulent crossflow is an equal mass exchange that does not produce a net flow change in either channel. If the enthalpies and velocities of the adjacent channels are different, however, a net exchange of energy and momentum will occur. The expressions for the net turbulent enthalpy flux, F_h , and momentum flux, F_m , from channel i to channel j are given, respectively, by

$$F_h = \frac{w'}{s} (h_i - h_j) \quad (5.29)$$

and

$$F_m = F_t \frac{w'}{s} (U_i - U_j) \quad (5.30)$$

where F_t is a correction factor to help account for the difference between energy and momentum turbulent transport.

The turbulent crossflow model can easily be related to the diffusion model by equating the expressions for turbulent energy flux, Equation (5.29), and diffusive energy flux. A finite difference expression for the diffusive energy flux

for the diffusive energy flux from channels i to j can be written as

$$F_h = \epsilon_t \rho (h_i - h_j) / \ell \quad (5.31)$$

where e_t is the eddy diffusivity and ℓ is the distance between channel centroids or other suitable mixing length. Equating Equation (5.31) to (5.29) yields

$$w' = \epsilon_t \rho \frac{S}{\ell} \quad (5.32)$$

The mixing factor, β , is related to e_t , by substituting Equation (5.27):

$$\beta = \frac{\epsilon_t}{\ell} \frac{\bar{\rho}}{\bar{G}} \quad (5.33)$$

where $\bar{\rho}$ is the average density of the adjacent channels. The same relationship follows from comparison of turbulent momentum flux definitions.

Besides direct input as a constant, three expressions for specifying β as a function of Reynolds number and geometry are

$$\begin{aligned} \beta &= a \text{Re}^b \\ \beta &= a \text{Re}^b \bar{D}_h / s \\ \beta &= a \text{Re}^b \bar{D}_h / \ell \end{aligned} \quad (5.34)$$

where a and b are input constants, $\bar{D}_h$ is the hydraulic diameter based on the sums of flow areas and wetted perimeters of the adjacent channels and

$$\text{Re} \equiv \bar{G}\bar{D}_h/\bar{\mu} \quad (5.35)$$

where $\bar{\mu}$ is the average viscosity.

A constant value or any of the expressions in Equations (5.34) can be used for β in two-phase flow if desired. Since two-phase mixing is strongly dependent on quality, however, β can also be specified as a tabular function of the quality which is calculated from the mixed mean enthalpy of the two subchannels.

6.0 APPLICATIONS

This section presents a variety of COBRA-IV applications. These include comparisons with exact solutions and experimental data performed for the purpose of code verification and additional computations to demonstrate COBRA's capability to consider important phenomena for which exact solutions or experimental data are not available.

Table 6-1 summarizes the computations contained in this section. These numerical simulations cover areas of interest to light-water reactors, both PWR and BWR, and the liquid metal fast breeder reactor. Computations are presented for steady-state and transient problems with single and two-phase flow, including examples representative of normal operating and accident analysis.

TABLE 6-1. Summary of COBRA Calculations

- 6.1 COBRA Comparisons with Analytic Solutions
 - Single-limb manometer
 - U-tube manometer
 - Two-phase flow decay
- 6.2 Data Comparisons
 - GE nine-rod bundle experiments
 - CE inlet jetting
 - W flow blockage
 - PNL flow blockage
 - Wire wrap
 - Application of COBRA for DNB Analysis
 - Semiscale core blowdown
 - Turbulent plane jet
- 6.3 Illustrational Computations
 - Isothermal PWR core oscillations
 - Heated PWR reflood
 - PWR core blowdown

6.1 COMPARISONS WITH ANALYTIC SOLUTIONS

Three COBRA comparisons to analytic solutions are presented in this section. These are:

- single-limb manometer
- U-tube manometer
- two-phase flow decay.

The first two simulations illustrate COBRA's capability to follow the motion of a steep density gradient as well as some of the code's new features. The third computation illustrates COBRA's capability to consider transient, one-dimensional two-phase flow.

6.1.1 Single-Limb Manometer

The first comparison between COBRA and an exact solution is for a single-limb manometer. Although this problem may be solved with several techniques, it is difficult to simulate using COBRA's Eulerian numerical mesh. The primary difficulty is the ability to compute the motion of very steep density gradients across fixed cell boundaries.

The equation of motion of the single-limb manometer problem was reduced to a system of first-order differential equations and solved numerically using a forth-order Runge-Kutta (R-K) scheme. This was considered the reference to which the COBRA code could be compared.

A frictionless single-limb manometer model, shown in Figure 6-1, was chosen to be 72 in. long with an initial liquid column of 45 in. An applied constant pressure was sufficient to support only 39 in. Therefore, due to the hydrostatic head/pressure imbalance, the system oscillates with a 2-sec natural period.

A small amount of damping and phase shift is evident in the COBRA-IV results presented in Figure 6-2. Some of the extraneous damping may be of a numerical nature inherent in the COBRA-IV solution algorithm. However, this damping tends

to be overridden when even a small amount of frictional drag is included, and computations for practical problems should not be affected.

FIGURE 6-1. Single-Limb Manometer Model

FIGURE 6-2. Undamped Single-Limb Manometer Results

6.1.2 U-Tube Manometer

An important feature of the COBRA-IV-I code is that lateral flows may be blocked at specific locations. The simulation of oscillations in a U-tube manometer illustrates this computational capability and serves as a prelude to coupled downcomer/core computations presented later.

The model, shown in Figure 6-3, consists of two 72-in. channels, each with 24 computational cells connected laterally through the lowest two cells. No flow is permitted through the bottom boundary. The channels are initially filled with saturated liquid to levels of 45 in. and 33 in., respectively, and the remaining volume contains saturated vapor. The imbalanced gravity head causes fluid oscillations to begin immediately.

To provide an "exact" solution for comparison, the equation of motion from the preceding section was modified for the U-tube case and also solved via the Runge-Kutta (R-K) scheme. Comparison of the COBRA and R-K results in Figure 6-4 shows trends similar to the single-limb case with generally quite good agreement, although some damping is again present in the COBRA predictions.

6.1.3 Flow Decay Transient

In two-phase flow systems, exact solutions are infrequent. Systems which do lend themselves to exact solution are usually simplified; however, it is still very useful to compare computed results with available exact solutions to two-phase flow systems.

An exact solution to a two-phase flow system was presented by Gonzalez-Santalo and Lahey (1972). In this work, the basic conservation equations for a one-dimensional homogeneous two-phase flow are presented and, with assumptions similar to those used in COBRA-IV, an exact solution is obtained for the case of an exponential inlet flow decay.

FIGURE 6-3. U-Tube Manometer Model

FIGURE 6-4. Undamped U-Tube Manometer Results

For comparison purposes, the equations were solved for a specific problem. The problem was that of a single channel characterized by:

- flow area, 0.2376 in.^2 ;
- heated length, 6 ft;

- constant heat flux, 3 million Btu/hr-ft²;
- system pressure, 1000 psia;
- saturated inlet enthalpy;
- exponential flow decay, $G_{\text{inlet}} = 1.0(10^6)e^{-0.333t}$.

The exact solution of quality as a function of time at two axial positions is shown in Figure 6-5 and the exact solution for the inlet and exit mass fluxes are shown as functions of time in Figure 6-6. COBRA results for this same case are also shown in Figures 6-5 and 6-6. The computations are in excellent agreement with the analytical solution.

FIGURE 6-5. Flow Decay Transient Quality Versus Time

FIGURE 6-6. Flow Decay Transient Mass Flux Versus Time

6.2 DATA COMPARISONS

This section presents the results of comparisons between COBRA simulations and experimental data. The problems considered are:

1. General Electric nine-rod bundle experiment
2. Combustion Engineering inlet jetting
3. Westinghouse flow blockage
4. PNL flow blockage
5. Wire-wrapped bundle
6. Application for DNB analysis
7. Semiscale core blowdown
8. Turbulent plane jet.

Table 6-2 describes the main parameters of each problem.

TABLE 6-2. Classification of COBRA-IV
Simulations for Data Comparison

<u>Problem</u>	<u>Steady State</u>	<u>Transient</u>	<u>Coolant</u>	<u>Single-Phase</u>	<u>Two-Phase</u>
1	X		Water	X	X
2	X		Water	X	
3	X		Water	X	
4	X		Water	X	
5	X		Sodium	X	
6	X		Water		X
7		X	Water		X
8	X		Water	X	

6.2.1 General Electric Nine-Rod Bundle Experiment

In these experiments (Lahey et al., 1970), measurements of the exit mass flow rate and enthalpy were made in representative side, corner, and center subchannels of a 3 x 3 rod bundle. Data were obtained for both adiabatic and diabatic conditions. Since the test section was biaxially symmetrical, the geometric model used in the COBRA-IV-I simulation was a 1/8 section of symmetry. Due to the large amount of data obtained during this experimental program, data comparisons will be presented only for representative test conditions to illustrate the predictive capability of the COBRA code.

For the adiabatic tests, the computed and experimental exit mass velocities are compared in Figure 6-7. In general, the agreement is good for all subchannels.

For the diabatic conditions, computed results for exit mass velocity and quality in the side, corner and central subchannels are compared with the experimental data in Figure 6-8. There is generally good agreement between the simulated and experimental results for the center and side subchannels. However, for the corner subchannel, the code predicts lower exit mass velocities and higher exit qualities than the experimental values.

The heated two-phase experiments illustrate a phenomenon of "lateral drift"--the preferential lateral movement of vapor toward regions of higher velocity which COBRA-IV does not model. Current development of the COBRA code includes the incorporation of drift flux models which may improve the code's ability to simulate the flow and quality distributions measured during these experiments.

FIGURE 6-7. Comparison of Measured Versus Calculated Subchannel Exit Mass Velocities for the Single-Phase Isothermal Data

FIGURE 6-8. Comparison of Measured Versus Calculated Subchannel Exit Mass Velocities for the Two-Phase Data

6.2.2 Combustion Engineering Inlet Jetting Tests

The objective of the CE inlet jetting experiments (Marshall and Letendre, 1968) was to investigate the flow development length for a nonuniform inlet velocity distribution in an unheated 15 x 15 square array rod bundle. The test section, shown in Figure 6-9, simulates the lower portion of a fuel assembly mounted on a core support plate. Coolant flowed through four holes in the support plate, producing a jetting effect at the inlet to the bundle. Velocity profiles were measured at various axial locations directly over the centerline of the jet and in a bundle row tangent to the jet boundary. The term jet boundary refers to an imaginary cylindrical surface projected upward from the base of a core support plate flow hole.

The COBRA simulation employed a symmetrical 1/8 section of the experimental rod bundle. Figure 6-10 describes this geometric model and illustrates the positions within the bundle where experimental velocity measurements were made.

FIGURE 6-9. Geometry of 15 x 15 Square Array Test Section

FIGURE 6-10. Subchannel Layout for CE Inlet Jetting Test

Results of the COBRA-IV simulation are compared with the experimental data in Figures 6-11 and 6-12. The COBRA computation is shown to be in excellent agreement with the experimental data.

6.2.3 Westinghouse Flow Blockage Tests

In the Westinghouse flow blockage experiments (Chelemer et al., 1973) the mass flow distribution in two adjacent open-lattice 14 x 14 rod bundles was measured at several axial levels. Several tests were run with different inlet mass flows in each bundle to simulate a partially (67 percent/33 percent) or completely (100 percent/0 percent) blocked inlet to one of the rod bundles.

The first data comparison is for the axial development of bundle average flow rate. For this case, it was sufficient to model the test section as two interconnected flow channels in the COBRA code, each having the flow area, wetted perimeter,

FIGURE 6-11. Inlet Jetting Test, Centerline Data

FIGURE 6-12. Inlet Jetting Test, Tangent Data

and hydraulic diameter of one rod bundle. The bundle flow distributions calculated using this representation are compared with the experimental data for the 67 percent/33 percent inlet flow distribution in Figure 6-13, and for the 100 percent/0 percent inlet flow distribution in Figure 6-14. Results of the simulation using COBRA-IV are in good agreement with the experimental data.

A more detailed representation of the test section was required to compare results obtained with COBRA-IV and the measured subchannel velocity profile. This model contained a strip of 29 channels, 14 for each bundle and one channel representing the region between them. The computed velocity profiles are compared with the 67 percent/33 percent inlet flow distribution experimental results in Figure 6-15. Again, the numerical simulation is in excellent agreement with the data.

6.2.4 PNL Flow Blockage Experiments

Experiments were conducted at PNL to determine axial velocity, turbulent intensity, and turbulent scale values in an unheated 7 x 7 rod bundle containing partial flow blockages (Creer et al., 1976). The experiment was undertaken to improve the understanding of flow distributions in partially blocked rod bundles during a loss-of-coolant accident, and to aid in verifying the capability of the COBRA computer code to perform flow blockage analyses.

Experiments were conducted using both water and air. The COBRA computations in this analysis simulate the water experiments. The water experiments were performed in a recirculating hydraulic loop using a 7 x 7 square array rod bundle containing sleeve blockages. The blockages, 3 in. long with 1-in. tapers at each end, simulated "ballooned" fuel rods with blockage severities of 70 and 90 percent in the center four subchannels.

FIGURE 6-13. Data for Inlet Flow Distribution of 67 Percent/33 Percent

FIGURE 6-14. Data for Inlet Flow Distribution of 100 Percent/0 Percent

FIGURE 6-15. Axial Velocity Profiles for Westinghouse Flow Blockage Data

Axial velocity profiles were measured at selected locations both upstream and downstream of the blockage using a laser Doppler anemometer (LDA). Data were obtained at Reynolds numbers of $1.44(10^4)$, $2.98(10^4)$, and $5.8(10^4)$, corresponding to bundle average velocities of 2.7, 5.7, and 10.7 ft/sec, respectively. Three geometrical arrangements were investigated: a 70 percent blockage located midway between two grid spacers, a 90 percent blockage located midway between two grid spacers, and a 90 percent blockage located immediately upstream of a grid spacer.

In this data comparison, the COBRA code was used to compute subchannel velocities for the three test geometries at $Re = 2.98(10^4)$. A full-length, 1/8 symmetrical cross section of the bundle was modeled as shown in Figure 6-16. The results of the COBRA simulation are compared with the experimentally measured values in Figures 6-17 through 6-19. The figures display the ratio of local velocity to bundle average velocity as a function of axial distance along the bundle. Note that in the COBRA calculations, the velocity is the average subchannel velocity, and the experimentally measured velocities are the centerline velocities. Experience indicates that the centerline velocity is generally 5 to 10 percent higher than the subchannel average, but such an adjustment in the data would not significantly affect the results as presented.

The simulated results are in good agreement with the experimental data. The jetting effect predicted by COBRA as occurring in the throat of the blockage could not be measured experimentally because geometrical constraints made it impossible to position the measuring volume of the LDA any closer than ± 1.3 in. from the blockage centerline. The 70 percent blockage simulation employed the steady-state implicit finite differencing scheme. This method went unstable when presented with the 90 percent blockage problem, and COBRA's transient explicit scheme was used.

FIGURE 6-16. COBRA Geometry Model

FIGURE 6-17. COBRA Velocity Predictions in Subchannel #1 with a 70 Percent Blockage

FIGURE 6-18. Ninety Percent Blockage Velocity Profile

FIGURE 6-19. Velocity Profile for a 90 Percent Blockage Adjacent to a Spacer

6.2.5 Wire Wrap Application

The application of the COBRA package to wire-wrapped LMFBR assemblies is demonstrated by comparing COBRA temperature calculations to measured temperatures in the ORNL 19-rod FFM-2A Test Bundle (Fontana et al., 1973). The COBRA input geometry along with other pertinent input is given in Figure 6-20. The data to which the comparison is made is from tests 020372-1054 and 022472-1143 which used a uniform power distribution. The results shown in Figure 6-21 are for a cross-diagonal traverse in which the measuring thermocouples are located in a rake 3 in. downstream of the end of the heated zone.

I. GEOMETRY

SUBCHANNEL TYPE	AREA (in. ²)	WETTED PERIMETER (in.)	ROD-ROD GAP (in.)	ROD WALL GAP
	0.0146	0.3613	0.056	-
	0.0296	0.6473	0.056	0.061
8	0.0093	0.1204	-	0.061

II. TURBULENT MIXING

$$\beta = 0.01$$

III. FORCED DIVERSION CROSS FLOW

$$\delta = 0.1033, P = 12 \text{ in.}$$

$$\frac{\delta P}{\Delta X} = 1.24$$

FIGURE 6-20. COBRA Input for ORNL-FFM-2A Test Assembly

FIGURE 6-21. Comparison of Calculated and Measured Normalized Exit Temperatures in the Uniformly Heated FFM-2A Test Assembly

6.2.6 Example of Application of COBRA to DNB Analysis

An important application of the COBRA subchannel analysis code is the comparison of experimental departure from nucleate boiling (DNB) data to empirical DNB correlations used in determining the design thermal margin for PWRs. Most such analyses performed with COBRA have involved proprietary data and/or correlations which are unavailable for general publication. However, an analysis was performed with data and correlations available in the open literature (Rosal et al., 1974) where DNB measurements were obtained using a 16-pin bundle with non-uniform radial and axial power distribution. Measurements were taken using thermocouples. A sudden rapid temperature excursion indicated by a thermocouple was considered evidence

of the occurrence of DNB, and the location of the thermocouple was considered to be the location of DNB. Because thermocouple locations were spaced 4 in. apart, some scatter would be expected in the data. The parameter ranges of the data were:

- system pressure: 1500, 1800, 2100, and 2400 psia
- inlet mass velocity: 1.5, 2.0, 2.5, 3.0, and $3.5(10^6) \text{ lb}_m/\text{hr-ft}^2$.
- average bundle power: 1.622 to 2.671 MW.
- inlet temperature: 476 to 615°F.

The characteristic parameter in DNB analysis is the Minimum Departure from Nucleate Boiling Ratio (MDNBR). This quantity is the minimum value of the ratio of the critical heat flux calculated using an empirical correlation, $q''_{\text{predicted}}$, and the locally measured heat flux, q''_{measured} . The COBRA subchannel analysis code is used to compute local thermal-hydraulic conditions in the bundle from the experimental parameters of pressure, inlet flow rate, bundle power, inlet enthalpy, and bundle geometry. The critical heat flux at each axial location is calculated from the thermal-hydraulic solution and a DNB correlation. The DNB ratio, $q''_{\text{predicted}}/q''_{\text{measured}}$, is calculated for each location, and the location of the MDNBR is considered to be the location of DNB. Ideally, the MDNBR would be exactly 1.0 for each data point, but in practice both the correlations and the data exhibit some scatter.

In this analysis, DNB calculations were performed for the same test condition using the Babcock & Wilcox B&W-2 DNB correlation and the Westinghouse W-3S DNB correlation. The range of the B&W-2 correlation extends only to pressures above 2000 psia, so this correlation was applied only for the

43 data points above 2000 psia. The W-3S correlation was evaluated for all 70 data points. The MDNBRs calculated with the B&W-2 correlation yielded a mean of 0.988, with a standard deviation of 0.149. The mean for the W-3S correlation was 0.873, with a standard deviation of 0.154. Figures 6-22 and 6-23 show that the distributions of the MDNBRs evaluated using each correlation are essentially normal about the mean. These results indicate that both the B&W-2 and W-3S correlations predict DNB well, for this set of DNB data, using the thermal-hydraulic solution from COBRA.

6.2.7 Semiscale Core Blowdown Calculations

The Semiscale facility is being used to experimentally investigate the system response to PWR loss of coolant accident conditions. The facility contains a core, pressure vessel, pump, steam generator and associated piping. The computations performed with the COBRA code modeled only the Semiscale core. The simulation considered the first 10 sec of blowdown for test S-02-3 (Crapo et al., 1975). Required boundary conditions and values for COBRA input parameters were supplied, whenever possible, from experimental results.

Figure 6-24 shows the axial representation used for the core. The model, 190 in. overall, considers the core from the lower plenum to the hot legs and contains a 65-in. electrical heated length with unheated portions above and below. Figure 6-25 displays a detailed description of the subchannel model of a 1/8 section-of-symmetry from the 40-rod core used in the computation. It consists of 6 rods and 6 interconnected flow channels to provide a multidimensional geometric representation of a symmetrical section of the Semiscale core.

FIGURE 6-22. Distribution of the MDNBR Values Calculated Using the B&W-2 DNB Correlation

FIGURE 6-23. Distribution of MDNBR Values Calculated Using the W-3S Correlation

FIGURE 6-24. Semiscale Core

FIGURE 6-25. Subchannel Model of the Semiscale Core

Computational boundary conditions for core pressure drop, system pressure and the enthalpy of fluid entering the core were determined directly from experimental measurements. Additionally, the rod heat flux was supplied from the results of an inversion calculation which utilized experimentally measured rod temperatures. Three results from this computation will be discussed:

- data comparisons for inlet density
- data comparison for inlet flow rate
- computed results for exit flow rate.

Figure 6-26 presents a comparison of the COBRA prediction and experimentally determined core inlet density and Figure 6-27 compares the computed and measured core inlet flow rate. In general, both show reasonable agreement. Unfortunately, uncertainties in some important boundary conditions make a detailed evaluation of the computed results impossible.

Flow measurements were not made at the core exit; it is therefore impossible to compare with experimental values at this location. However, it is important to understand the flow behavior at this location so the computed exit mass flux for subchannels 1 and 5 are presented in Figure 6-28. Although some variations are evident, the calculated flow behavior is, as expected, primarily one-dimensional.

6.2.8 Turbulent Plane Jet

Although COBRA is usually applied to problems where the major shear stresses are at solid boundaries and fluid-fluid shear is relatively minor, as in a rod bundle geometry, the code can be applied to many two-dimensional problems in a fluid continuum. To illustrate this capability, a simulation of a turbulent plane jet was performed.

FIGURE 6-26. Comparison of Experimental and Calculated Core Inlet Density

FIGURE 6-27. Comparison of Experimental and Calculated Inlet Mass Flow Rate

FIGURE 6-28. Calculated Exit Mass Flow Rate

By applying mixing length theory to the boundary layer equations, Schlichting (1968) determined that the width of a two-dimensional plane turbulent jet issuing from a point source is directly proportional to distance along the jet centerline and the centerline velocity is inversely proportional to the square root of the distance. In addition, the eddy viscosity has been determined experimentally to be $\epsilon = 0.037 bU$ where b is the jet half-width and U is the local centerline velocity.

For a two-dimensional jet issuing from a slot of width B_0 , Albertson et al. (1948) showed that an axial zone of flow

establishment exists from the slot out to a distance of about $5.2 B_o$. In this zone the velocity profile undergoes the transition from uniform at the slot to a normal Gaussian distribution at the end of the zone.

To model this transition region with COBRA, the code was modified slightly to use two expressions for turbulent mixing. In the zone of flow establishment,

$$\epsilon = 0.037 B_o \frac{X}{S} V_X$$

Outside the transition zone,

$$\epsilon = 0.037 B_o \left[\frac{(X-s)}{B_o} + 1 \right] V_X$$

where $s = 5.2 B_o$ is the length of the transition zone and V_X is the local velocity. The use of these correlations should yield a centerline velocity decay inversely proportional to the square root distance beyond the transition zone.

This expected behavior is compared to the COBRA computation in Figure 6-29. Because it is not possible to exactly simulate a free jet with COBRA, a direct quantitative comparison cannot be made. Nevertheless, the centerline velocity decay predicted by COBRA is quite close to the inverse square root variation. The velocity field shown in Figure 6-30 reveals a roughly Gaussian distribution and clearly shows the entrainment of surrounding fluid.

Steady state was achieved by running a transient until velocity variations became small. This required a 1.25 sec transient, or about 6 jet transit times at inlet velocity. A computation time of 65 sec was required on a CDC7600 for 432 cells and 300 time steps.

FIGURE 6-29. Turbulent Plane Jet Centerline Velocity Decay

FIGURE 6-30. Velocity Vector Field for Turbulent Plane Jet

6.3 ILLUSTRATIONAL COMPUTATIONS

This section describes the results of COBRA calculations for problems of importance to the nuclear community to illustrate some of the expanded capability of the COBRA code. The simulations presented are:

- isothermal PWR core oscillations
- heated PWR reflood
- PWR core blowdown.

6.3.1 Isothermal Reflood Oscillation

This demonstration problem was performed to investigate multidimensional effects of isothermal PWR core oscillations by comparing the response of a PWR core with a uniform initial water level in the core to a system with a nonuniform initial liquid level.

The geometry for this problem was constructed to represent a full-size PWR core, including downcomer and plenums. The actual modeling setup for this problem is shown in Figure 6-31. The downcomer is modeled by one channel connected to the outer core channel at the bottom two cells. The annular arrangement of the core was chosen to provide core channels of equal area and heated perimeter. Drag coefficients are included at the core inlet and exit to simulate inlet and exit hardware. At the core exit, a loss coefficient of 700 was used to represent the hydraulic resistance of the primary coolant system from the upper plenum through the steam generator, pump, and piping out to a postulated break.

A comparison of the liquid level in the downcomer and core channels for the cases of uniform and nonuniform initial liquid levels is presented in Figures 6-32 and 6-33. Note that the downcomer level oscillations of the two cases are nearly identical even though individual core channels oscillate

RADIAL NODING

AXIAL NODING

FIGURE 6-31. PWR Core Model Showing Nonuniform Core Liquid Level

FIGURE 6-32. Water Level Oscillations with Uniform Initial Core Level

FIGURE 6-33. Water Level Oscillations with Nonuniform Initial Core Level

quite differently. The secondary oscillations within the core, caused by the initial nonuniform core mass distribution, are strongly damped within a few cycles but the primary motion of the total mass of the coupled core and downcomer is unaffected by secondary motion in the core. It is apparent that, for the isothermal case, the overall motion of the system is determined by the amount of mass in the system, not by its distribution within the core.

6.3.2 Heated Reflood Oscillation

This sample problem extends the preceding isothermal reflood simulation by including heat addition via the incorporation of a fully-coupled fuel rod model. The objective is to evaluate the effect of a cosine versus uniform radial core power distribution on heated reflood oscillation phenomena. The core geometry used for this problem is identical to the isothermal case.

At the start of the transient, a steady-state fuel rod temperature distribution is evaluated with decay power and adjusted rod surface boundary conditions to give an average surface cladding temperature of approximately 1100°F. An initially uniform liquid level fills the lower plenum to the bottom of the core. After a short period to allow the core steam temperatures to stabilize, subcooled water is introduced to the lower plenum, reaching an equivalent core flooding rate of about 6 in./sec at 0.7 sec.

The overall core dynamic behavior and clad temperature response for 25 sec are presented in Figures 6-34 through 6-36. Figure 6-34 shows the liquid level in the downcomer and core, and the core axial velocity profile. The temperature response is described in Figure 6-35, which shows the

FIGURE 6-34. Liquid Level and Velocity, Uniform Power

FIGURE 6-35. Heat Transfer, Uniform Power

FIGURE 6-36. Axial Temperature Profile, Uniform Power

clad temperature, surface heat transfer coefficient and density for the first foot of core in each of the four core flow channels. Figure 6-36 displays the axial surface temperature profiles for the inner and outer rods in the first four feet of the core. Only the uniform power case is shown, since the nonuniform case is similar.

The general system behavior for this time period appears to consist of two fairly distinct stages. The first is characterized by a violent, chaotic oscillation and a net decrease in the amount of liquid in the lower plenum. The second state, characterized by somewhat better behaved oscillations, begins after a particularly violent expulsion at 8-1/2 sec which overflows the downcomer and nearly empties the lower plenum. Note that the beginning of the second stage corresponds roughly with the time when most of the fuel rods in the first foot of core have cooled nearly to saturation temperature. During this later period, liquid refills the lower plenum and penetrates the first few inches of the core.

A periodic reverse flow of steam in the outer channel affects the core temperature distributions at later times. Figure 6-37 shows core temperature contours at 0 and 25 sec for the uniform radial power case and 0, 25, and 50 sec for the cosine radial power profile. Note that the outer channel remains somewhat hotter in the uniform case and that the shape of the lower temperature contours in the nonuniform power case are flatter at 25 and 50 sec than initially.

These results cannot be considered as typical PWR reflood behavior. Since this simulation was performed mainly as a test of the hydraulic solution scheme, a blowdown heat transfer correlation set was used as it was readily available in the code but recognizing that reflood heat transfer correlations would be required for a true simulation. The use of one-foot computational cells in conjunction with the blowdown

FIGURE 6-37. Transient Core Temperature Contours

heat transfer logic caused the "stepwise" quenching observed in these results. This nonphysical process is so violent that the true response of the flow field is probably obscured. A reflood heat transfer model is under development to remedy this problem.

6.3.3 PWR Blowdown Calculations

Numerical simulations of coolant behavior in a representative PWR core during the blowdown portion of a LOCA were undertaken to investigate the significance of multidimensional flow redistributions during blowdown. The effects of core radial power distribution on the flow redistributions were examined. The effect of a regional flow blockage was investigated in a second calculation.

The COBRA model of the PWR core consisted of a 1/8 sector of the core with 6 flow channels and 14 axial nodes. Figure 6-38 illustrates a lateral cross section of the PWR sector and the geometric representation used in COBRA for these calculations. Boundary conditions required for the computation were obtained from the results of a RELAP-4 calculation. These are similar to those used in the Semiscale computations, except that the COBRA fuel rod conduction model was used here instead of specifying the surface heat flux as was done in the previous case.

Results for the blowdown simulation without flow blockage are shown in Figures 6-39 through 6-41. Figures 6-39 and 6-40 are the computed inlet and exit mass flux for flow channels 1 and 6. Figure 6-41 shows a flow field vector display of normalized mass flux during the initial core flow reversal. The blowdown transient is initiated from steady-state normal operating conditions, and all flows are positive at time $t = 0$. By 0.126 sec, a flow stagnation plane is beginning to form and an important flow redistribution,

FIGURE 6-38. Model of PWR Geometry
for COBRA Calculations

FIGURE 6-39. Calculated Inlet Mass Velocities
for Channels 1 and 6

FIGURE 6-40. Calculated Exit Mass Velocities
for Channels 1 and 6

FIGURE 6-41. Calculated Flow Field in the PWR Core During the Blowdown Transient

caused by nonhomogeneous voiding in the hottest regions of the core, forces fluid toward the cooler outer periphery. By approximately 0.25 sec, the system pressure has dropped sufficiently so that void production is more homogeneous throughout the core and the flow pattern tends toward one-dimensional behavior. Also, a plane of stagnation is evident near the midline of the core, where water flashing to steam causes coolant to be forced out both ends of the core. Results at 0.5 sec are similar to those at 0.25 sec but with lower flow rates. Finally, at 0.66 sec all flows are negative and, again, very nearly one-dimensional.

Although the contributions of flow redistribution may be important during initial depressurization, these calculations indicate that PWR blowdown hydrodynamics are primarily one-dimensional, controlled by core-wide phenomena, particularly voiding, with relatively small flow redistributions caused by the radial power profile. It is important to note, however, that these calculations were made with the assumed boundary condition of uniform pressures at the core inlet and exit, and indicate only that the radial power distribution by itself is probably not responsible for major flow redistributions.

The second PWR blowdown simulation incorporates all conditions present in the first, with the addition of a flow blockage. The blockage used in this computation does not necessarily represent the type or magnitude of blockage expected during a LOCA; it was arbitrarily selected for this simulation solely to investigate the qualitative character of possible multidimensional flow redistribution. This blockage was introduced only in Channel 1 and it is present for the entire computation, i.e., it is not introduced as a function of time. The flow area remains constant at the nominal value from the core inlet to an axial position of 6 ft. Between 6 and 7 ft the area of Channel 1 is reduced by 40 percent, and

between 7 and 8 ft the flow area expands back to the nominal value. The fuel rod conduction model was not modified to include effects of rod swelling. The only impact of the blockage on heat transfer characteristics would be through changes in thermal-hydraulic parameters contained in heat transfer correlations.

Figure 6-42 presents a comparison of a normalized velocity flow field at 0.0 sec for the blocked and unblocked cases, respectively. The normalization factor is different for the two plots and meaningful comparisons of vector length can be made only within each figure. The relative angle of the vectors from the vertical can be compared meaningfully between the two figures, however.

It is evident that the blockage disturbs the nominal flow field. Fluid is forced out of Channel 1 in the vicinity of the blockage, with subsequent flow recovery downstream. Flow redistributions in the vicinity of the blockage during blowdown are qualitatively similar to those shown for steady state. Although a blockage of this magnitude causes local flow redistributions, the overall character of blowdown in this simulation remains controlled by void production. Thus, the blockage does not change the general hydraulic characteristics calculated for the PWR blowdown simulation without the blockage.

FIGURE 6-42. Normalized Velocity Flow Field for PWR Core
With and Without an Arbitrary Flow Blockage

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APPENDIX

CONNECTION MATRIX EXAMPLES

APPENDIX
CONNECTION MATRIX EXAMPLES

A. CONNECTIONS

Interchannel Connections			Rod-Channel Connections			Wall-Channel Connections		
No.	Chan.	Chan.	No.	Rod	Chan.	No.	Wall	Chan.
1	1	2	1	1	1	1	1	2
2	1	3	2	1	2	2	1	5
3	1	4	3	1	4	3	2	3
4	2	3	4	2	1	4	2	6
5	2	4	5	2	2	5	3	4
6	3	4	6	2	3	6	3	7
7	5	6	7	3	1			
8	5	7	8	3	3			
9	6	7	9	3	4			
$N_k = 9$			$N_{kr} = 9$			$N_{kw} = 6$		

B. MATRIX ELEMENTS

Channel No.

$$[D_c] = \begin{matrix} & \overbrace{\begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{matrix}} & \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{matrix} & \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix} & \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{matrix} \end{matrix} \left. \vphantom{\begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{matrix}} \right\} \begin{matrix} \text{Channel} \\ \text{Connection} \\ \text{No.} \end{matrix}$$

Channel No.

Rod No.

$$[D_r] = \begin{matrix} & \overbrace{\begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{matrix}} & \overbrace{\begin{matrix} 1 & 2 & 3 \end{matrix}} & \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{matrix} & \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & -0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} & \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{matrix} \end{matrix} \left. \vphantom{\begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{matrix}} \right\} \begin{matrix} \text{Rod-Channel} \\ \text{Connection} \\ \text{No.} \end{matrix}$$

Channel No.

Wall No.

$$[D_w] = \begin{matrix} & \overbrace{\begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{matrix}} & \overbrace{\begin{matrix} 1 & 2 & 3 \end{matrix}} & \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{matrix} & \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1- & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1- & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1- & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1- & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1- & 0 & 0 & 1 \end{bmatrix} & \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{matrix} \end{matrix} \left. \vphantom{\begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{matrix}} \right\} \begin{matrix} \text{Wall-Channel} \\ \text{Connection} \\ \text{No.} \end{matrix}$$

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