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COMMIX-1C: A Three-Dimensional Transient Single-Phase Computer Program for Thermal-Hydraulic Analysis of Single-Component and Multicomponent Engineering Systems

User's Guide and Manual

Prepared by H. M. Domanus, Y. S. Cha, T. H. Chien, R. C. Schmitt, W. T. Sha

Argonne National Laboratory

Prepared for U.S. Nuclear Regulatory Commission

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Prepared by H. M. Domanus, Y. S. Cha, T. H. Chien, R. C. Schmitt, W. T. Sha

Argonne National Laboratory 9700 South Cass Avenue Argonne, IL 60439

Prepared for Division of Systems Research Office of Nuclear Regulatory Research U.S. Nuclear Regulatory Commission Washington, DC 20555 NRC FIN A22550

List of Contributors

At the request of and under sponsorship from the U.S. Nuclear Regulatory Commission, the COMMIX-1C computer code was constructed by refining selected features from previous COMMIX versions and adding innovations. The task of making COMMIX-1C available and useful was a team effort, and the participants are listed below according to their activities.

Documentation: Y. S. Cha, R. C. Schmitt, W. T. Sha, and

H. M. Domanus

Previous COMMIX versions: H. M. Domanus, R. C. Schmitt, and W. T. Sha

Software Design, Models, and Methods: H. M. Domanus and R. C. Schmitt

Code Programming and Development: H. M. Domanus, R. C. Schmitt, and T. H. Chien

Validation: H. M. Domanus, T. H. Chien, Y. S. Cha, and

W. T. Sha

Overall Project Direction and

Management: W. T. Sha

COMMIX-1C: A Three-Dimensional Transient Single-Phase Computer Program for Thermal-Hydraulic Analysis of Singleand Multicomponent Engineering Systems

Volume II: User's Guide and Manual

Abstract

The COMMIX-1C computer program is an extended and improved version of previous COMMIX codes with four major additions or modifications: (1) a new finite-volume formulation for the mass, momentum, and energy equations to extend the applications to subsonic compressible flows and to make the calculations more robust: (2) a flow-modulated skew-upwind discretization scheme to reduce numerical diffusion; (3) two new matrix solvers for the discretized equations to increase the flexibility and efficiency of numerical computation; and (4) a k-\varepsilon two-equation turbulence model that is more robust and better validated than those in previous COMMIX codes. In addition, there are numerous smaller modifications that improve overall operation greatly.

COMMIX-1C solves the conservation equations of mass, momentum, and energy, as well as the transport equations of turbulence parameters. It is designed to perform steady-state/transient, single-phase, three-dimensional analysis of fluid flow with heat transfer in a single-component or a multicomponent engineering system. The program was developed for the analysis of heat transfer and fluid flow processes in a nuclear reactor system. However, it is designed in a generalized fashion so that, with little or no modification, it can be used to analyze processes in any engineering equipment or in any system.

The following are unique features of the COMMIX-1C code:

- Porous-Medium Formulation: COMMIX-1C uses a new porous-medium formulation with the parameters of volume porosity, directional surface porosity, distributed resistance, and distributed heat source or sink. With this formulation, the COMMIX code has the capability to model an anisotropic flow domain with stationary structures, and it can be used to treat irregular geometries. The porous-medium formulation with the additional parameter of directional surface porosity represents a unified approach to thermal-hydraulic analysis. Because of this feature, it is now possible to perform a multidimensional thermal-hydraulic simulation of either a single component, such as a rod bundle, reactor plenum, piping system, or heat exchanger, or of a multicomponent system that is a combination of such components.
- Three Matrix Solvers: In COMMIX-1C, three matrix solvers, the successive
 overrelaxation method, the Yale Sparse Matrix Package, and the preconditioned conjugate gradient method for symmetric matrix, are available to solve
 the pressure equation and scalar transport equations. Depending on the size
 of the computational domain, the user can choose the solver that is best

suited for a given problem. These three matrix solvers greatly increase the flexibility and efficiency of numerical computation for COMMIX-1C compared to previous COMMIX codes.

- Geometrical Package: A special geometrical package has been developed and implemented to permit modeling of any complex geometry in the most storage-efficient way.
- Skew-Upwind Discretization Scheme: A new flow-modulated skew-upwind discretization scheme has been developed and implemented to reduce the numerical diffusion observed in simulations of flow inclined to grid lines.
 The scheme also eliminates temperature over/undershoots that occur when simulations are performed with other skew-upwind differencing schemes.

Volume I (Equations and Numerics) of this report describes in detail the basic equations, formulations, solution procedures, and models for auxiliary phenomena. Volume II (User's Guide and Manual) contains the input instruction, sample problems, flow charts, and description of available options and boundary conditions.

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Executive Summary

The COMMIX (Component Mixing) codes are designed for analyzing heat transfer and fluid flow. The COMMIX-1C computer program—an extended version of previous COMMIX codes—is designed to analyze steady-state/transient, single-phase, three-dimensional flow with heat transfer in a reactor component/multicomponent system.

The four major improvements that have been implemented in previous COMMIX codes (including COMMIX-1B) to develop COMMIX-1C are

- New inite-volume formulation for the mass, momentum, and energy equations to extend application to subsonic compressible flows. The new momentum formulation employs the concept of a volume-averaged velocity. It makes the numerical calculation more robust than in previous COMMIX versions. It also makes the location of pressure change coincide with that of density change for one-dimensional flows. In addition, the new discretized momentum equations also satisfy the one-dimensional Bernoulli equation.
- Addition of a new flow-modulated skew-upwind discretization scheme in the
 energy equation to reduce numerical diffusion. This new scheme is considered better than the previous volume-flow-weighted skew-upwind
 difference scheme in COMMIX-1B because it not only reduces numerical
 diffusion but also has a theoretical basis for not producing overshoots and
 undershoots that are physically unrealistic.
- Addition of two matrix solvers, the Yale Sparse Matrix Package and the
 preconditioned conjugate gradient method, for the solution of discretized
 equations. These two new matrix solvers, plus the existing solver using the
 successive overrelaxation method, greatly enhance the flexibility and
 efficiency of COMMIX-1C in dealing with various engineering problems.
- An improved k-ε two-equation turbulence model that is more robust and better validated than that in previous COMMIX codes.

In addition to these major improvements, there are numerous minor modifications that significantly improve the overall operation.

One of the major unique features of COMMIX is its porous-medium formulation, which has been rigorously derived through local volume averaging. In the new formulation, we use volume porosity, directional surface porosity (directional because surface porosity is an anisotropic vector quantity), distributed resistance, and distributed heat source or sink. The concept of adding the parameter of directional surface porosity is relatively new. In the conventional porous-medium formulation, only the volume porosity, distributed resistance, and distributed heat source are used. Volume porosity is the ratio of the volume occupied by fluid in a control volume to the total control volume. Surface porosity is similarly defined as the ratio of fluid flow area through a control surface to the total control surface area. The porous-medium formulation has the capability of modeling both the anisotropic flow domain and irregular geometry.

In any numerical analysis of an engineering system, modeling must include distributed resistance (friction factor) because, in general, it is not a precisely known quantity. Thus, with the conventional porous-medium formulation, the flow distribution that we obtain depends completely on how accurately we model the distributed resistance. However, in the case of the present porous-medium formulation, due to the introduction of directional surface porosity (a geometrical quantity that can be prescribed accurately), the dependence of the velocity field on resistance modeling is reduced. Hence, we obtain improved resolution and accuracy in the modeling of velocity and temperature fields. The present porous-medium formulation thus represents the first unified approach to thermal-hydraulic analysis. The conventional porous-medium formulation can be considered a subset of this present porous-medium formulation.

The COMMIX code provides detailed local velocity and temperature fields for the problems under consideration. The conservation equations of mass, momentum, and energy and the transport equations of turbulence parameters are solved as a boundary-value problem in space and an initial-value problem in time. The discretization equations are obtained by integrating the conservation equations over a control volume.

The code has a wide range of applicability. It is capable of solving thermal-hydraulic problems involving either a single component, such as a rod bundle, reactor plenum, piping system, heat exchanger, etc., or a multicomponent system that is a combination of these components.

COMMIX has two alternative solution schemes. One is semi-implicit and is a modification of the ICE technique. The other, a fully implicit scheme called SIMPLEST-ANL, is a modification of the numerical procedure known as SIMPLER.

The code has a modular structure and permits analysis with either Cartesian or cylindrical coordinate systems. It has four thermal-hydraulic property packages: water vapor, sodium vapor, liquid sodium, and liquid water. Besides these four packages, an option is available for users to input simplified thermal-physical property correlations that are valid in the desired range of applications.

Another unique feature of the COMMIX code is its geometrical package. The basic concept is to use computational cells (either in Cartesian or cylindrical coordinates) as building blocks that are stacked to approximate the shape of the physical systems under consideration. Then volume porosity and directional surface porosity are used to account for the differences between the geometry used in computation and the actual configuration. This feature permits the COMMIX code to model any irregular and complex geometry encountered in a real engineering system. Furthermore, the computer storage requirement of the COMMIX code is optimized; only the computational cells used in calculations are counted.

Volume I (Equations and Numerics) of this report describes in detail the basic equations, formulation, flow-modulated skew-upwind discretization scheme, and solution procedures. It also describes models used for the following phenomena:

- · Momentum interaction between fluid and stationary solid structures.
- · Thermal interaction between fluid and stationary solid structures.

· k-ɛ two-equation turbulence model.

In Volume II (User's Guide and Manual), we provide flow charts, descriptions of subroutines, geometry modeling, initialization procedures, input descriptions, etc. Two sample problems are also included so that readers who plan to use COMMIX-1C can become familiar with the input/output structures of the code.

1 Introduction

1.1 Purpose

COMMIX (for Component Mixing) is a computer code for analysis of heat transfer and fluid flow. Since the development of COMMIX-1 in 1976, many features have been added and/or refined to augment the code's applicability. Consequently, COMMIX has become a very general-purpose computer code with a very wide range of applications. Although developed for nuclear reactor applications, COMMIX can be used with little or no modification to analyze various processes in engineering systems.

Many industries and organizations involved in the design or analysis of nuclear reactors are already using COMMIX. However, due to the code's generality of formulation and its wide range of applications, individuals in other disciplines have also found COMMIX a very useful tool. We therefore expect the number of COMMIX users to increase in the future. Prospective users of COMMIX can benefit from a comprehensive description of the code. The purpose of the present report is to meet this need.

In describing COMMIX-1C, we have two distinct aims. One is to convey to the reader the capabilities of COMMIX, the equations that are solved and how they are solved; this was done in Volume I of this report. The second aim is to present a step-by-step procedure on the use of COMMIX. To achieve this, we must describe the procedure with sufficient detail so that a reader has little or no lifficulty in beginning to use COMMIX. This, of course, is not an easy task, but we have attempted it here in Volume II.

It may be stressed here that while extending previous COMMIX versions to COMMIX-1C, we have retained the original structure and format of COMMIX. Therefore, provious COMMIX users will have little difficulty in adapting and running their problems with the COMMIX-1C version.

Volume I. Equations and Numerics, describes the basic equations, formulations of discretization equations, auxiliary models, solution procedures, etc. Volume II, User's Guide and Manual, describes all information needed by the user, e.g., input description, flow chart, sample problems, and user options.

1.2 Organization of the Report

This volume describes the step-by-step procedure in sufficient detail so that a reader unfamiliar with the COMMIX code can begin to use it with little difficulty.

We begin in Sec. 2 by describing the overall structure of the program. The first step for a user beginning numerical simulation is to model the geometry. Therefore, in Sec. 3 we describe the geometrical conventions of COMMIX, recommend modeling procedures, and suggest how to prepare geometry-related input for COMMIX.

After geometrical modeling, a user should initialize cell and boundary values. COMMIX has several boundary-condition options that a user can select. These are described in Sec. 4.

If a flow domain under investigation contains solid structures, there will be thermal and momentum interaction between fluid and solids. The modeling of thermal interaction (between fluid and structures) through thermal structures is presented in Sec. 5. The force-structure modeling to account for momentum interaction between fluid and structures is presented in Sec. 6.

In COMMIX-1C, we have implemented two solution schemes (fully implicit and semi-implicit) and three matrix solvers (successive overrelaxation method. Yale Sparse Matrix Package, and preconditioned conjugate gradient method). The user can select any combination of the solution schemes and the matrix solver for a given problem so that the convergence rate and computation efficiency can be increased. The preparation of input related to solution scheme and matrix solver is described in Sec. 7.

Auxiliary input such as turbulence modeling, flow-modulated skew-upwind difference scheme, and simplified property is presented in Sec. 8.

COMMIX requires an initial steady-state calculation, either for analysis of a steady-state problem or to obtain an initial condition for a transient simulation. All input required for steady-state calculation is described in Sec. 9. The details related to transient simulations are presented in Sec. 10.

In Sec. 11, we describe the input/output procedures and all related variables. Section 12 contains final concluding remarks.

Appendix A, *Input Description*, contains what will be for many users the most valuable part of the whole report, for it is there that all input variables are described. In Appendix B, we list all subroutines and their functions; Appendix C contains a list of resistance correlations.

Two sample problems, along with their description, input, and output, are presented in Appendices D and E. These problems were selected to provide a good introduction to the capabilities of COMMIX-1C.

2 Structure of COMMIX-1C

2.1 Overall Flow Chart

The overall street of the computer program can be seen from the flow chart presented in Fig. 1. The major steps of the program are as follows:

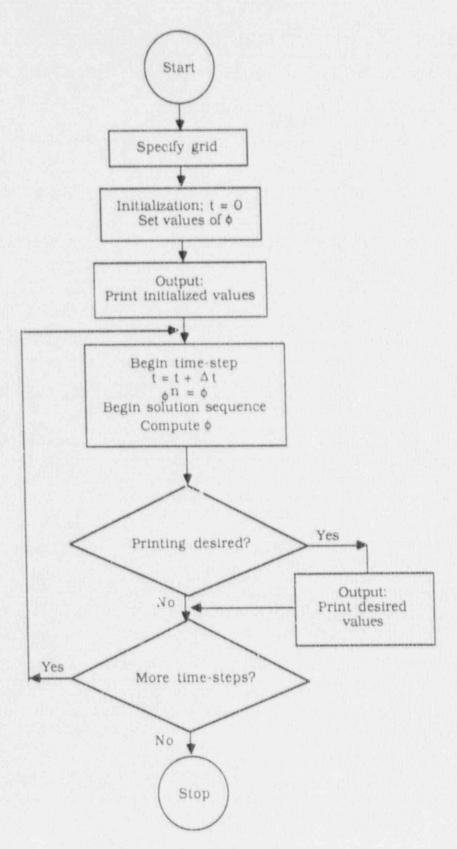


Fig. 1. COMMIX-1C flow chart

- We begin numerical simulation by specifying the grid and calculating all
 geometrical quantities that are needed frequently in later work. Reading of
 geometry input is done in subroutine GEOM3D. Calculation of all geometrical
 quantities is done in the subroutine BOXES, which includes both the
 Cartesian and the cylindrical coordinate systems.
- Next, the initial values of all variables are either specified or calculated. The
 subroutine INITAL is the main subroutine for initialization. It sets up the
 default values, reads NAMELIST/DATA, and calls appropriate subroutines
 (see Table 1 for reading input data, calculating initial values, and printing, if
 desired, of input and control parameters).
- After completion of initialization, subroutine OUTPUT is called to print initial values of all desired variables.
- The solution sequence, for which further details are given below, is then
 performed to determine the value of all dependent variables at the new time.
 Subroutine TIMSTP determines the sequence of calling subroutines,
 required during the solution sequence. When the values of all variables at the
 new time are determined, we return to the main subroutine AMAIN.
- If printing is desired at this time, subroutine OUTPUT is called and desired variables are printed.
- If the required number of time steps have been performed, or the maximum computation time or the maximum real time is reached, then computation is terminated and, if requested, the restart data are written on disk file.
 Otherwise, old time values are updated and execution continues for the next time step.

2.2 Solution Sequence

The flow diagram of the solution sequence controlled by the subroutine TIMSTP is shown in Fig. 2. This subroutine TIMSTP can be considered as the heart of the program. It performs what we call an outer iteration loop.

There are three major subroutines called by the subroutine TIMSTP:

- Mass-Momentum Loop: Mass-momentum equations are solved and new values of velocities and pressures are computed. Subroutine MOLOOP calls required subroutines in sequence to solve the mass-momentum equations.
- Turbulence Loop: Two subroutines, TKLOOP and TDLOOP, are called to calculate the turbulence parameters k (turbulence kinetic energy) and ϵ (rate of dissipation of k). Turbulent viscosity and conductivity are then calculated by calling the subroutine TURV12.
- Energy Loop: The energy equation is solved and new values of enthalpy are calculated. Subroutine ENLOOP calls appropriate subroutines in sequence to solve the energy equation.

Table 1. Initializing subroutines

	In	put Data	Function or	
Subroutine	NAMELIST	RECORDS	Parameters Initializes	
INITAL	GEOM DATA		Initializes default values and calls initializing subroutines	
INFORC	DATA	Force-structure	Force-structure parameters	
INPSTR	STRUCT T F M	Thermal-structure prototype and location records	Thermal-structure parameters	
1CTEMP	DATA		Boundary values of velocity, temperature, heat, density, and pressure	
BARIN		Boundary and initial value records	Boundary and initial values of pressure, velocity, tempera- ture, enthalpy, heat source, porosity, and surface area	

The mass-momentum and energy loop program subroutines are discussed in more detail in Secs. 2.3 and 2.4. The turbulence loop is discussed in Sec. 8.

2.3 Mass-Momentum Loop

The flow chart of the mass-momentum loop, as described below, is shown in Fig 3. The calling sequence is performed in the subroutine MOLOOP.

- First, calculate the pressure-velocity-relation coefficients û, ŷ, ŵ, du, dv, and dw described in Secs. 4 and 5 of Vol. I. These calculations are performed in subroutines XMOMI, YMOMI, and ZMOMI for x (or r), y (or θ), and z directions, respectively.
- Using these pressure-velocity-relation coefficients, calculate the coefficients of pressure equation, a_0^p , a_1^p , a_6^p , b_0^p (see Table 16 of Vol. I) in subroutine PEGN.
- The pressure equation is then solved in subroutine SOLVER by one of the matrix solvers (subroutine SOLVIT for the successive overrelaxation method, subroutine YSMP for the Yale Sparse Matrix Package, and subroutine CGRAD for the preconditioned conjugate gradient method). If the successive overrelaxation method or the preconditioned conjugate gradient method is selected by the user, the solution is performed with an iterative procedure.

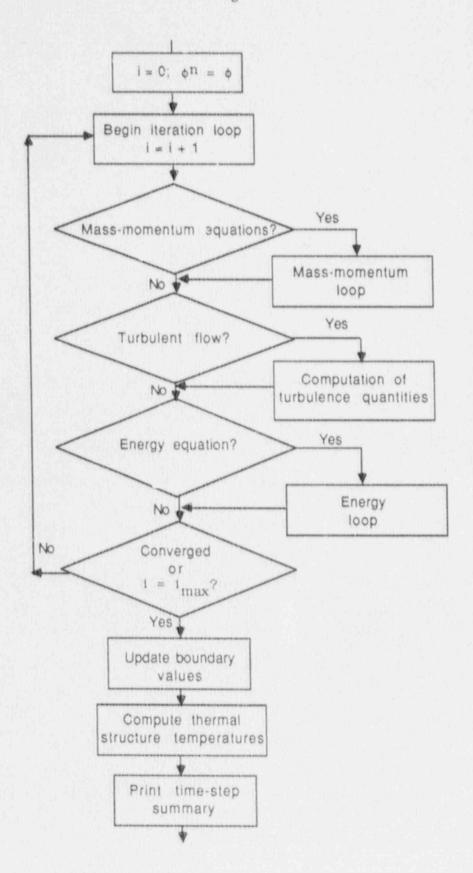


Fig. 2. Flow chart of solution sequence in subroutine TIMSTP

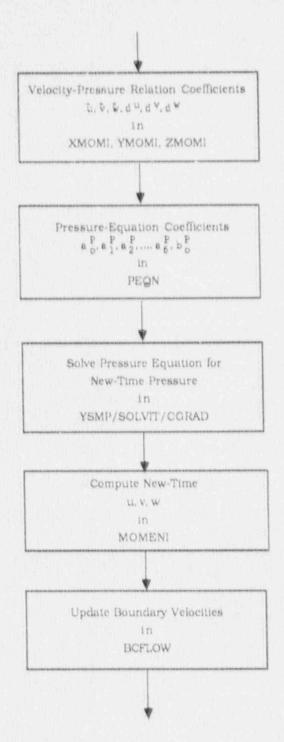


Fig. 3. Flow diagram of mass-momentum loop

The iteration is continued until either the residue of the pressure equation is below the specified convergence criterion value or the number of iterations has reached the specified maximum value, called ITMAXP. If the Yale Sparse Matrix Package is selected, the solution is obtained by direct inversion and no iteration is involved.

 Velocities are then updated in subroutine MOMENI using the new pressure values and the following relations:

$$\begin{split} u &= \hat{u} - d^{u} (\delta p_{2} - \delta p_{0}), \\ v &= \hat{v} - d^{v} (\delta p_{4} - \delta p_{0}), \text{ and} \\ w &= \hat{w} - d^{w} (\delta p_{6} - \delta p_{0}). \end{split}$$

Finally, update the velocity boundary values in subroutine BCFLOW.

This completes the mass-momentum loop.

2.4 Energy Loop

The sequence of computations in the energy loop (the calling sequence is performed in subroutine ENLOOP) is shown in Fig. 4.

- · First, update the boundary values in subroutine BCTEMT.
- · Compute the source terms in subroutine ESORCE.
- Compute the convective fluxes in subroutine ENCONV.
- Compute the diffusion fluxes and energy equation coefficients in subroutine ENERGI.
- If the implicitness parameter $\alpha > 0$, go to subroutine SOLVER and solve the energy equation

$$a_0^h h_0^{n+1} = \sum_{\ell} a_{\ell}^h h_{\ell}^{n+1} + b_0^h$$

for new-time enthalpy values by either the successive overrelaxation method (subroutine SOLVIT) or the Yale Sparse Matrix Package (subroutine YSMP).

If $\alpha = 0$ (semi-implicit procedure), compute new-time enthalpy values using the old-time values of the neighboring points, i.e.,

$$a_0^h h_0^{n+1} = \sum a_\ell^h h_\ell^n + b_0^h$$

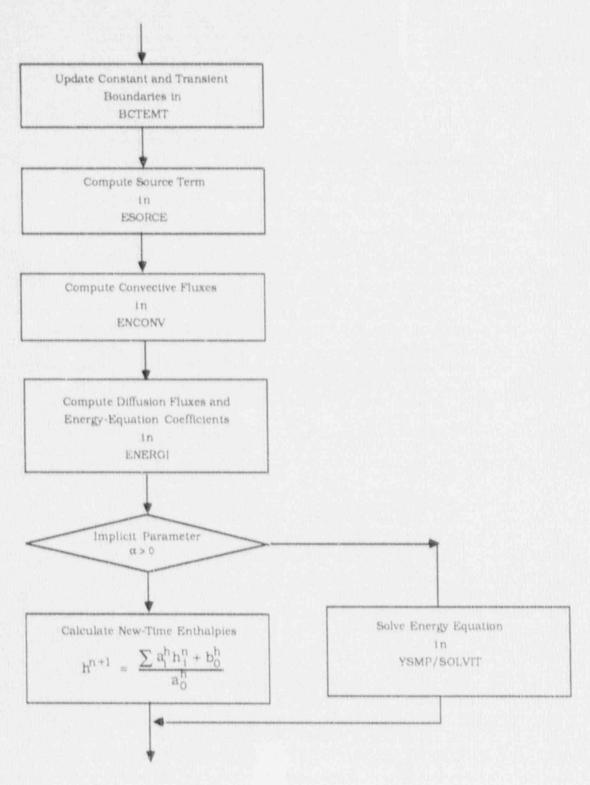


Fig. 4. Flow diagram of energy loop

3 Geometry Modeling

3.1 Introduction

In most cases, the first step for every user is to model the geometry of the system to be simulated. The geometry concept of COMMIX is somewhat unique, and is different from the conventional approach. However, we are confident that after using the COMMIX geometry package, the user will not only feel at ease with the COMMIX concept, but will begin to appreciate the benefits of the COMMIX approach. To make the acquaintance period as easy and smooth as possible, we recommend that all new users read this section with particular attention.

3.2 Concept and Definitions

In numerical modeling, a computational flow domain is always partitioned into a number of computational cells by means of x, y, and z grid planes in a Cartesian coordinate system or by r, θ , and z in a cylindrical system, as shown in Fig. 5. In COMMIX, we use the conventions described below to define various elements of a flow domain. A simple box geometry, shown in Fig. 6, is taken as an illustration.

Computational Cell

In COMMIX, the computational cell is defined by the location of cell-volume faces with the grid point placed in the geometrical center of the cell. Cell sizes can be nonuniform. A computational cell surrounded only by other computational cells is called an internal cell. If one cell surface is a boundary surface, it is called a boundary cell. A user must specify the total number of computational cells required through the FORTRAN variable NM1.

· Boundary Surface

The external boundaries enveloping the flow domain are called the boundary surfaces. These may be solid walls or planes through which fluid can flow. The geometry in Fig. 6a has eight boundary surfaces.

A boundary surface is defined by its unit normal vector. The x, y, and z components (XNORML, YNORML, and ZNORML) of a unit normal vector are specified so the vector points locally into the fluid region. In Fig. 6a, the normal vector of surface 2 has components (-1,0,0). Table 2 illustrates the components of the unit normal vectors of eight surfaces of the geometry in Fig. 6a.

· Regular Surface

A boundary surface coincident with any one of the grid planes is called a regular surface. The geometry of Fig. 6 has all regular surfaces.

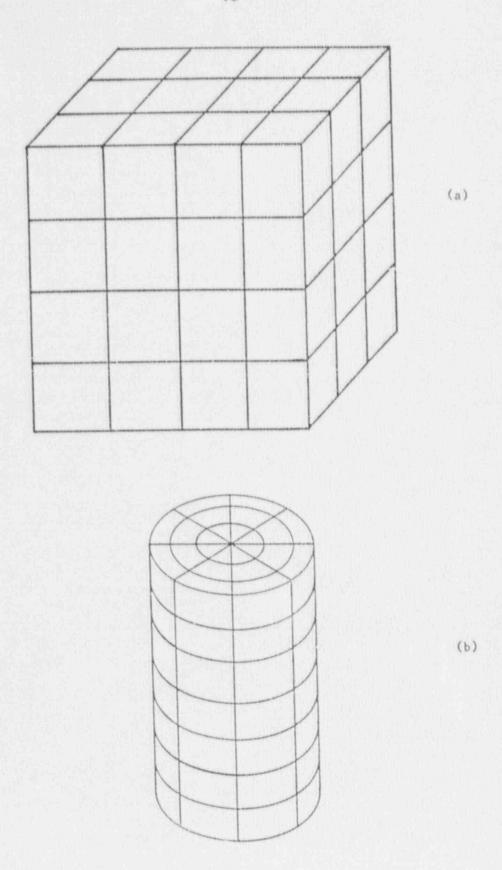
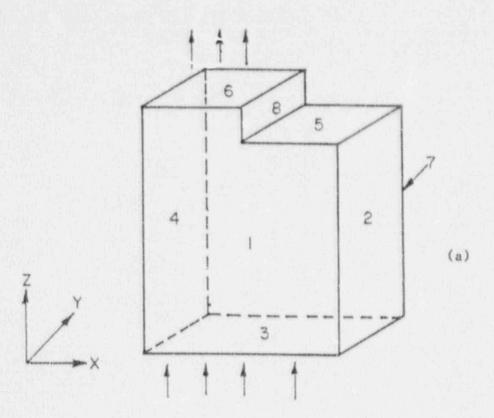


Fig. 5. Partitioning in (a) Cartesian coordinate system and (b) cylindrical coordinate system



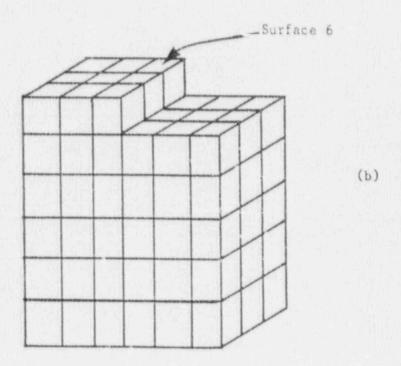


Fig. 6. (a) Model geometry showing boundary surfaces; (b) partitioning of a model geometry showing surface elements

Table 2. Components of unit normal vectors of geometry in Fig. 6a

Surface	XNORML	YNORML	ZNORML
1	0	1	0
2	-1	0	0
3	0	0	1
4	1	0	0
5	0	0	-1
6	0	0	-1
7	0	-1	0
8	-1	0	0

· Irregular Surface

A boundary surface noncoincident with any grid plane is called an irregular surface. In Fig. 7a, surface 1 is an irregular surface. Note that only regular surfaces can be specified as inlet and outlet planes. In other words, flow thlet and outlet cannot be trregular surfaces.

· Surface Number

A user must give a surface number to every boundary surface. The same surface number can be assigned to all boundary surfaces that have

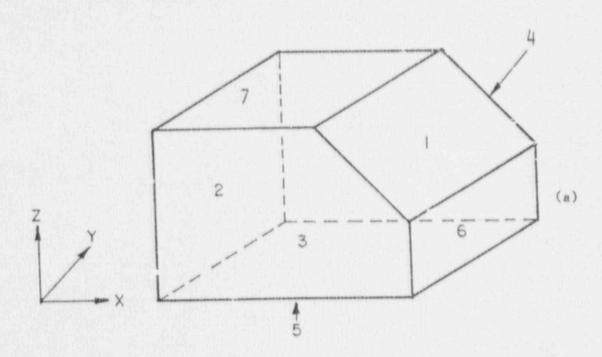
-The same unit normal vector and

-The same velocity, pressure, temperature, and heat flux boundary conditions.

For example, surfaces 2 and 8 in Fig. 6a are in two different planes. However, we can assign them the same surface number if they both have the same unit normal vector and same boundary conditions, as illustrated in Fig. 8. Of course, one can also define them as two different surfaces if desired.

If surfaces 3 and 8 have different boundary conditions, as illustrated in Fig. 9, we must consider them as two different surfaces, even though the surfaces may be coincident and have the same unit normal vector.

The variable NSURF is used to specify a total number of surfaces. Note that all tregular surfaces must be numbered before other regular surfaces are numbered.



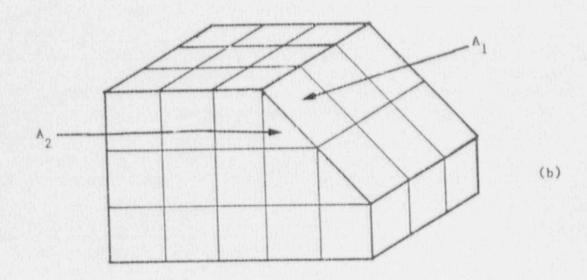


Fig. 7. Model geometry showing (a) trregular surface and (b) partitioning and surface elements

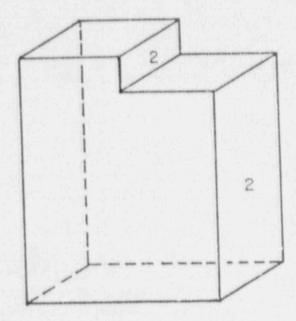


Fig. 8. Two noncoincident surfaces with the same surface number

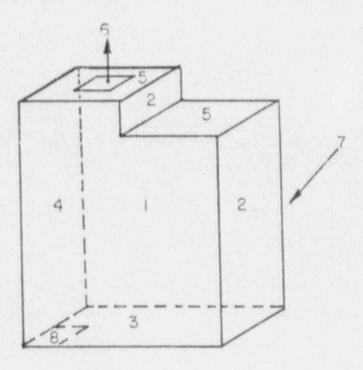


Fig. 9. Two coincident surfaces with different surface numbers

· Irregular Cell

If one surface of a computational cell is an irregular surface, that cell is called an irregular cell. An irregular cell cannot be an interior cell because an irregular cell contains an irregular surface that is part of a boundary surface. Note that a computational cell is permitted to have only one irregular surface.

· Surface Element

A section of a surface between two pairs of consecutive grid lines is defined as a surface element. A surface can therefore have more than one surface element. For example, in Fig. 6b, surface 6 has nine surface elements. The variable NL1 is used to specify the total number of surface elements.

· Volume Porosity

The geometrical parameter called volume porosity γ is defined as the ratio of fluid volume in a cell to the total cell volume. The FORTRAN variable name for volume porosity is AL and its numerical value must lie between 0 and 1. This parameter is included to account for (1) irregularity in geometry and (2) the existence of internal solid structures. For example, the volume porosity of the computational cell due to irregular geometry (Fig. 10a) is

$$\gamma = AL = \frac{\Delta x \, \Delta y \, \Delta z - volume \ of \ prism \ A}{\Delta x \, \Delta y \, \Delta z} \, .$$

Similarly, the volume porosity due to an internal solid structure (Fig. 10b) is

$$\gamma = AL = \frac{\Delta x \, \Delta y \, \Delta z \, \cdot \, volume \, \, of \, half \, solid \, cylinder}{\Delta x \, \Delta y \, \Delta z} \, .$$

· Directional Surface Porosity

Similar to volume porosity, the directional surface porosity γ_i is defined as the ratio of fluid flow area to total surface area. Because γ_i is a directional quantity, we have three surface porosities. The variable names are ALX, ALY, and ALZ for the κ (or r), y (or θ), and z directions, respectively. For example, in Fig. 10a,

$$\begin{split} \gamma_X(i+1/2.j,k) &= ALX \; (\text{cell ijk}) = (\Delta y \Delta z - \text{area A1})/(\Delta y \Delta z), \\ \gamma_Y(i.j+1/2,k) &= ALY \; (\text{cell ijk}) = 1.0, \; \text{and} \\ \gamma_Z(i.j,k+1/2) &= ALZ \; (\text{cell ijk}) = (\Delta x \Delta y - \text{area A3})/(\Delta x \Delta y), \\ \text{and in Fig. 10b,} \end{split}$$

$$\begin{split} \gamma_X(i+1/2,j,k) &= \text{ALX (cell ijk)} = (\Delta y \Delta z - \text{area A5})/(\Delta y \Delta z), \\ \gamma_Y(i,j+1/2,k) &= \text{ALY (cell ijk)} = 1.0, \text{ and} \\ \gamma_Z(i,j,k+1/2) &= \text{ALZ (cell ijk)} = (\Delta x \Delta y - \text{area A4})/(\Delta x \Delta y). \end{split}$$

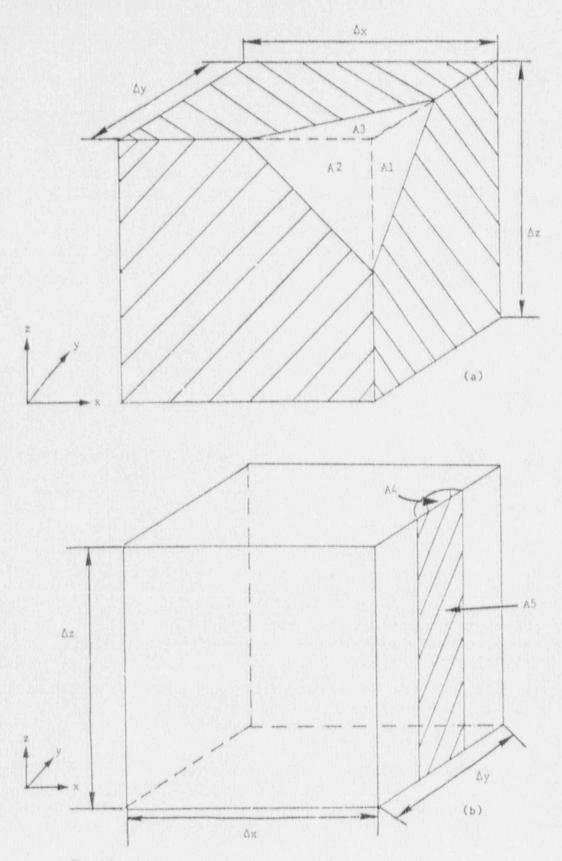


Fig. 10. Volume porosity due to (a) trregular geometry and (b) internal solid structure

We must mention here that the directional surface porosity is considered a flow-variable parameter. In the staggered grid arrangement, we define flow-variable parameters at the face of a cell. Therefore, when we describe γ_x , γ_y , and γ_z of cell (i.j.k), we mean γ_x at (i+1/2.j.k), γ_y at (i.j+1/2.k), and γ_z at (i.j.k+1/2).

3.3 Recommended Approach

The task of developing a geometrical model of a flow domain represents

- · Selection of an appropriate coordinate system,
- Partitioning of a computational flow domain into a number of computational cells by means of coordinate grid planes, and
- Computation of geometrical partition sizes.

The development of a geometrical model of a physical situation requires an artful balance between an attempt to represent the geometry as accurately as possible on the one hand, and minimizing the computational cost in terms of time and storage on the other hand. This ger erally places an upper limit on the number of computational cells. The model must therefore try to balance homogenization of the details and accuracy in the factors that affect fluid flow and heat transfer.

Developing a model and preparing input for a complex geometry involves many decisions. There is no clear-cut procedure in modeling, because most of the decisions to be made are problem-dependent. The user must follow his/her own intuition and judgment. The following are only broad suggestions:

- · Take advantage of symmetry and model the minimal required geometry.
- Determine if the geometry to be modeled is amenable to Cartesian or cylindrical coordinates and use the appropriate coordinate system.
- If large variations in parameters or properties are expected in certain regions of the computational domain, then finer meshes should be used in these regions.
- Relatively coarse mesh is recommended at the beginning to ensure that the input is correct and the results are reasonable. Then the mesh size should be doubled to determine the accuracy of the solution.

3.4 Geometry Input

After all major questions relating to geometry modeling have been answered, we can start preparation of geometry input. Below is a recommended step-by-step procedure.

· Specify value of the variable IGEOM.

IGEOM = 0 for Cartesian geometry and = -1 for cylindrical geometry.

 Partition the flow domain to be modeled by x, y, and z, or r, θ, and z grid planes. Fig. 11 illustrates some examples. Compute and specify the following:

IMAX, JMAX, and KMAX: Maximum number of cells in x, y, and z (or r, $\theta,$ and z) directions.

DX, DY, and DZ: Partitioning distances in x, y, and z directions.

NSURF: Total number of surfaces.

NM1: Total number of computational cells.

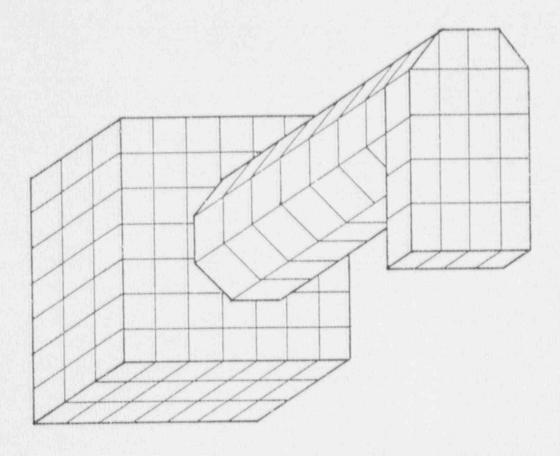
NL1: Total number of surface elements.

- Be sure to take advantage of the parameters IFX, IFY, and IFZ for one- and two-dimensional calculations. For example, if the system variables are independent of the x (or r for cylindrical coordinate) direction, set IFX = 0.
 The code will bypass all calculations that are x (or r) dependent.
- Give surface numbers to all boundary surfaces. Compute and specify XNORML, YNORML, and ZNORML (the components of unit normal vectors) for all surfaces. Note that all irregular surfaces must be numbered first. Partitioning must be done so that each cell has a maximum of one irregular surface.
- Compute areas of (1) surface elements of all irregular surfaces (such as surface area A₁ in Fig. 7b), and (2) partially truncated regular surface elements of irregular cells (such as surface area A₂ in Fig. 7b). Prepare and supply all information relating to surface elements, as described in the section on "Boundary Surface Identification Records" in the Input Description.
- Compute volume porosity AL and directional surface porosities ALX, ALY, and ALZ and input this information according to the section on "Cell Initialization Records" in Appendix A (Input Description).

4 Initialization

4.1 Introduction

After completing the geometrical modeling, we must assign initial values of temperature, pressure, and velocity to all cells and surfaces. If we are continuing a previous run, this initialization is performed through the restart capability of COMMIX.



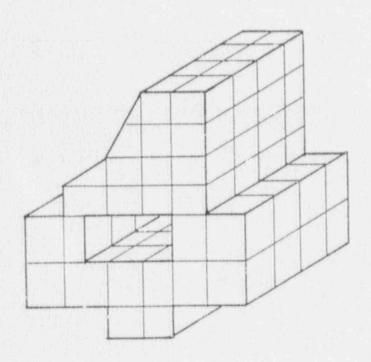


Fig. 11. Illustrations showing partitioning of sample geometries

The input of all initial and boundary values at the start of the first run can generally be very tedious. In COMMIX, we have provided several simplified input procedures that simplify initialization.

Lists of initialization variables for uniform and nonuniform conditions are given in Tables 3 and 4, respectively. The variables for nonuniform initialization override those for uniform initialization. For a more detailed description, please refer to Appendix A.

4.2 Simplified Procedures

- In the initial input, we need to specify only the values of temperature, pressure, and velocity. The values of enthalpy and density are not required; they are calculated in the code from the equation-of-state and the prescribed pressure and temperature distributions.
- We can prescribe initial hydrostatic pressure distributions in the entire flow domair, by specifying only
 - -One pressure value (variable name PRESØ).
 - -Its x, y, and z location (variables are XPRESØ, YPRESØ, and ZPRESØ), and
 - -The components of the gravity vector (variables are GRAVX, GRAVY, and GRAVZ).

The program then calculates the entire pressure field.

- Uniform temperature distribution in the entire flow domain can be obtained by specifying only one temperature value to the variable TEMP∅.
- Uniform temperature and hydrostatic pressure distributions can be overridden by using cell initialization records for desired (i.j.k) locations.
- The normal velocity and temperature for each surface, if uniform over a surface, can be prescribed by specifying desired values to variables VELOC(N) and TEMP(N), respectively, where N is the surface number. Uniform pressure at cells adjacent to a surface is specified by PRES(N) and only needs to be specified for a surface with the uniform pressure boundary condition.
- Nonuniform velocity and temperature distributions for surface elements can
 be specified by using the surface element initialization records with variables
 VELB and TLB. This overrides any VELOC(N) and TEMP(N) values.
 Nonuniform pressure distributions at cells adjacent to a surface having a
 specified pressure boundary condition is done using cell initialization
 records and overrides the PRES(N) specification.
- If surface heat flux instead of temperature is desired to be prescribed initially, it can be done by specifying the desired value to the variable TE'AP(N), which now has the units W/m². A nonuniform heat flux distribution can be specified by using the surface element initialization records with variable QBN. This overrides any TEMP value.

Table 3. Variables for uniform initialization

Variable	Variable Name	Initializing Region	Input Section	Remarks
remperature, °C	TEMPØ	Internal cell	DATA	One value for all cells
	TEMP(N)	Boundary surface	DATA	One value for each surface
Velocity, m/s	VELOC(N)	Boundary surface	DATA	One value for each surface
Pressure, Pa	PRESØ	Internal cell	DATA	Hydrostatic pressure distribution
	PRES(N)	Boundary surface	DATA	One value for each surface
Heat flux, W/m ²	TEMP(N)	Boundary surface	DATA	One value for each surface
Mass flux. $\frac{kg}{s-m^2}$	VELOC(N)	Boundary surface	DATA	One value for each surface

- From the prescribed initial temperature and pressure fields, initial values of density and enthalpy fields are computed by the code using the equation-ofstate.
- Turbulence parameters (k and ε) can be specified for internal cells and surface elements by using cell initialization records and the surface element initialization records with variables TK, TKB, TD, and TDB.
- Mass flow rates corresponding to uniform mass flux can be specified by VELOC(N).
- Mass flow rate can be specified for boundary surface by using the surface element initialization records with the variable FLOW. This overrides any value specified through VELOC.
- The form of the cell initialization records (CIR) and the surface element initialization records (SEIR) is

NAME RVAL IB IE JB JE KB KE N°

^{&#}x27;N for SEIR only.

Table 4. Variables for nonuniform initializationa

Variable	Variable Name	Initializing Region	Input Section	Remarks
Temperature, °C	TL	Internal cell	CIRb	Desired internal cells
	TLB	Surface element	SEIRC	Desired surface elements
Velocity, m/s	UL, VL, WL	Internal cell faces	CIR	Desired internal cell faces
	VELB	Surface element	SEIR	Desired surface elements
Pressure, Pa	POLD	Internal cell	CIR	Desired internal cells
Heat flux, W/m^2	QBN	Surface element	SEIR	Desired surface element
Enthalpy, J/kg	HL	Internal cell	CIR	Desired internal cells
	HLB	Surface element	SEIR	Desired surface elements
Density, kg/m ³	RLB	Surface	SEIR	Desired surface elements
Heat source, W/m ³	gsou	Internal cell	CIR	Desired internal cells
Turbulence kinetic energy, J/kg	TK	Internal cell	CIR	Desired internal cells
	TKB	Surface element	SEIR	Desired surface elements
Turbulence dissipation rate, W/kg	TD	Internal cell	CIR	Desired internal cells
	TDB	Scrface element	SEIR	Desired surface elements
Mass flow rate. kg/s	FLOW	Surface element	SEIR	Desired surface elements

aVariables listed in Table 4 override those listed in Table 3.

bCIR: Cell Initialization Records.

SEIR: Surface Element Initialization Records.

For example: The surface element initialization record

TLB 60.0 5 18 7 12 1 1 5

means that we are specifying a surface-temperature value of 60°C for all surface elements on computational cells having an I value from 5 to 18, J value from 7 to 12, and K value from 1 to 1 for surface number 5. We can see here that one input card in this example initializes the temperature value for 84 surface elements.

Similarly, the cell initialization record

TL 60.0 5 18 7 12 1 6

means that we are specifying a cell-temperature value of 60°C for all internal cells in the region having an I value from 5 to 18, J value from 7 to 12, and ¹⁵ value from 1 to 6. A total of 504 cells are initialized by this example card.

Before a program reads the input data, all variable values are made zero.
 Consequently, only the values other than zero need to be specified in the input data.

The commonly occurring values of variables are provided as default values. If the default value for a given variable is acceptable, the input for that variable need not be specified.

4.3 Input Preparation

4.3.1 Internal Cell Variables

In the input preparation of initial cell values, we must specify the values of the following variables:

Three Component Velocities UL, VL, and WL in m/s

- -Temperature TL in °C.
- -Pressure POLD in Pa, and
- -Heat source QSOU in W/m3.

As mentioned above, we must specify only the nonzero values.

If we have uniform temperature and hydrostatic pressure distributions at the start, we can make use of the simplified procedures and specify only TEMPØ and PRESØ in NAMELIST/DATA/.

In regard to the heat source, the user has the option either to use volumetric heat source QSOU or to specify it through thermal structures (see Sec. 5).

4.3.2 Boundary Surface Variables

· Types of Boundary Conditions

In boundary value initialization, we need to specify the type of boundary, as well as the boundary values. The variables used for defining the types of boundary conditions are:

KFLOW:

for velocity.

KTEMP:

for temperature/heat flux, and

KPRES:

for pressure.

The types of boundary conditions are listed in Tables 5-7. Details and description of these options are given in Volume I and Appendix A.

· Boundary Values

If a given boundary surface has a uniform value of velocity, temperature, or pressure, we can use variables VELOC(N), TEMP(N), or PRES(N) to initialize it. These values are specified in NAMELIST/DATA/.

If nonuniform boundary conditions are required, the input is performed through surface element initialization records (SEIR). Table 8 lists eight variables that can be specified through SEIR. In general, we need not specify all eight variables. Of course, one can always specify uniform boundary conditions by using the SEIR.

5 Thermal-Structure Modeling

5.1 Introduction

The purpose of implementing a thermal-structure model in COMMIX is to permit consideration of heat-transfer interaction between fluid and structures. The model implemented in COMMIX solves one-dimensional heat conduction equations for all solid structures. It calculates temperature distribution in solids and heat transfer from solids to surrounding fluids. In summary, the output from the thermal-structure model is a heat source/sink term for the fluid energy equation.

The basic equations, formulations, and features of the model are described in Volume I. Here, we describe only the user-related aspects of the model.

5.2 Some Concepts and Definitions

A thermal structure is a solid structure in a fluid-flow domain having heat-transfer interaction with surrounding fluid. It can be planar, cylindrical, or spherical. The COMMIX-1C model permits a structure axis to be aligned with only one of the three coordinate axes, as shown in Fig. 12. For a given flow domain, we can model as many the rural structures as desired.

Table 5. Options for velocity boundary conditions

Parameter KFLOW(N)	Boundary Condition Type	Physical Boundary	Remarksa
-5	Continuative mass	Outlet	$v_n^0 = \frac{(\rho A V)^{Al}}{(\rho A)^0}$ (one outlet surface element)
-4	Uniform velocity outlet	Outlet	$v_n^0 = \frac{\Sigma(\rho A v)^{Al}}{\Sigma(\rho A)^0}$ (several outlet surface etaments)
-3	Free slip	Symmetry	$v_n^0 = 0$, $\frac{\partial v_1^0}{\partial n} = 0$ No momentum
		surface	diffusion
-2	Continuative velocity outlet	Outlet	$v_n^0 = v_n^{Al}$ For constant density and area
-1	Continuative momentum outlet	Outlet	$v_n^0 = \frac{(\rho v)^{Al}}{\rho^0}$ For constant area
0	No slip	Stationary solid wall	$v_{ti}^0 = 0; v_t^0 = 0$
1	Constant velocity	Inlet, solid wall	$v_0^i \neq 0, v_1^i = 0$ $v_0^i = 0, v_1^0 = 0$
2	Constant mass flow rate	Inlet/ outlet	Mass flow rate specified by FLOW in the surface element initialization records
100 + NF	Uniform transient velocity	Inlet	$v_n^i(t) = VELOC(N)f(t)$ f(t) = Transient function number
200 + NF	Uniform transient mass flow rate	Inlet	FLOW(t) = VELOC(N) f(t)

^{*}Superscripts: 0 = Outlet or boundary value; Al = adjacent internal cell; i = inlet value; n = normal to boundary surface; t = tangential to boundary surface.

Table 6. Options for temperature/heat flux boundary conditions

Parameter KTEMP(N)	Boundary Condition Type	Physical Boundary	Remarks
1	Constant temperature	Inlet, solid wall	Tw = constant, qw is calculated
100 + NF	Transient temperature	Inlet, solid wall	$T_{w}(t) = T_{w}(0)f(t)$ q_{w} is calculated
200	Constant heat	Solid wall	Qw = constant. Tw is calculated
300 + NF	Transient heat	Solid wall	$q_w(t) = q_w(0)f(t)$. T_w is calculated
400	Adiabatic	Outlet, symmetry	$q_w = 0.0$

Table 7. Options for pressure boundary conditions

Parameter KPRES(N)	Boundary Condition	Physical Boundary	Remarks
0		-	No pressure boundary
1	Constant pressure	Inlet-outlet	condition is applied
100 + NFa	Transient pressure	Inlet-outlet	$P_w = constant$ $P_w(t) = P_w(0) F(NF)a$

aNF is the transient function number; F(NF) is the NFth transient function.

Table 8. Variables that can be specified through SEIR

		AND RESIDENCE AN
Variable	FORTRAN Input Names	Unit
Enthalpy Mass flow rate Heat flux Density Temperature Normal velocity Turbulence kinetic	HLB FLOW QBN RLB TLB VELB TKB	J/kg kg/s W/m² kg/m³ °C m/s J/kg
energy Turbulence dissipation rate	n TDB	W/kg

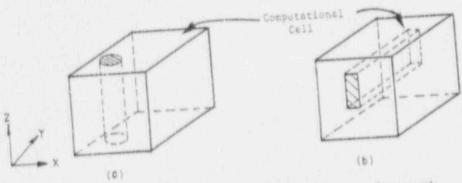


Fig. 12. Illustrations showing thermal-structure alignment:

- (a) cylindrical structure aligned to z axis;
- (b) plane si ucture aligned to y axis

A Thermal structure is identified by its unique geometric and physical features, i.e.,

- · All solid structures taving the same grid axis alignment, same geometric features, and same physical characteristics, even though spread out in a physical doma n, can be considered as one thermal structure, e.g., fuel pins in a nuclear reactor, flow tubes in a heat exchanger.
- · One solid structure with the same geometric features but not the same physical features throughout cannot be modeled as one thermal structure. e.g., a fuel pin having different material composition in different axial sections.

In COMMIX-1C computations, each thermal structure is partitioned by grid planes normal to the structure axis to Torm several thermal structure elements, as shown in Fig. 13. Each element has its own internal temperature distribution because the heat conduction equation is solved for each element.

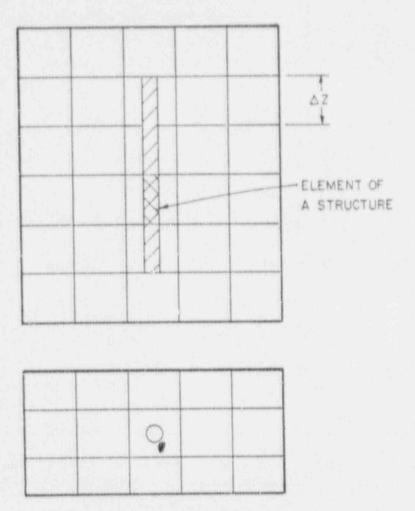


Fig. 13. An element of a thermal structure

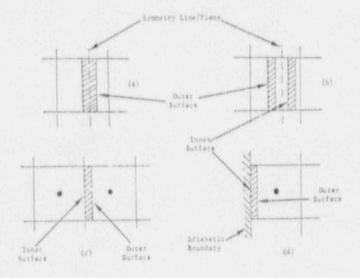


Fig. 14. Element of a thermal structure, showing outer and inner surfaces

A thermal structure has two surfaces, outer and inner. The inner and outer surfaces can be adiabatic or can interact with fluid, as shown in Fig. 14. Each element surface is permitted to interact only with one fluid cell. However, a fluid cell can interact with more than one element surface. This can be seen in Figs. 15 and 16.

Each structure can be composed of several material segments. Figure 17 illustrates the cross section of a structure element having

- . Outside and inside surfaces, numbered 1 and 2, respectively,
- · Three different materials separated by gaps, and
- · Each material region divided into a number of partitions.

5.3 Thermal-Structure Subroutines

There are three major subroutines related to the thermal-structure model:

- HSTRUC: Computes heat transfer coefficients for outer and inner surfaces of all thermal-structure elements. It uses local velocities for Reynolds number and appropriate user-specified heat transfer correlations to evaluate the heat transfer coefficient.
- QSTRUC: Solves the heat conduction equations for each element and computes the heat source term for the fluid energy equation.
- TSTRUC: Solves the heat conduction equations for each element and computes thermal-structure element temperature distribution.

The other three subroutines for this model are TSCAN, INPSTR, and PSTRUC. The functions of TSCAN are to scan input and determine storage requirements; INPSTR reads thermal-structure input and assigns appropriate markers and pointers; and PSTRUC prints results related to thermal structures.

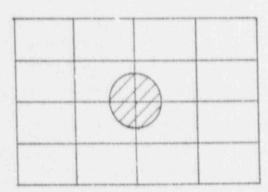


Fig. 15. Four quarter-cylindrical structures, each interacting with one fluid cell

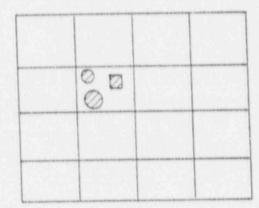
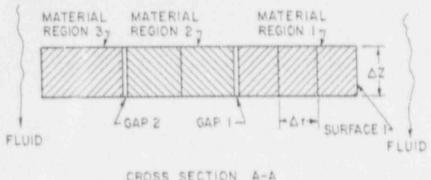


Fig. 16. Multiple structures interacting with a single fluid cell



CROSS SECTION A-A

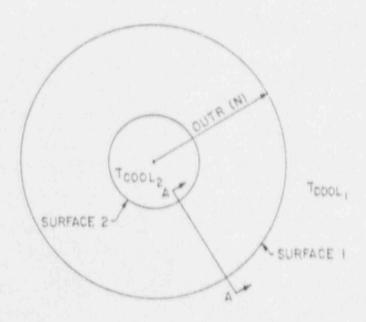


Fig. 17. Typical structure element showing material regions and gaps

5.4 Modeling Recommendations

The following is a list of recommendations relating to thermal-structure modeling:

- · For a steady-state analysis, we need to model only those solid structures with heat sources.
- · For a transient analysis, all solid structures, with or without heat source, must be modeled.
- · Only plane, cylindrical, or spherical shapes are permitted in COMMIX-1C. If a structure does not conform to one of these shapes, the user should exercise some approximations.
- . COMMIX-1C permits modeling of any multiple or fraction of a structure as one thermal structure; e.g., if there are 10 fuel pins passing through computational cells (Fig. 18a), we can consider the fuel pin as a thermal

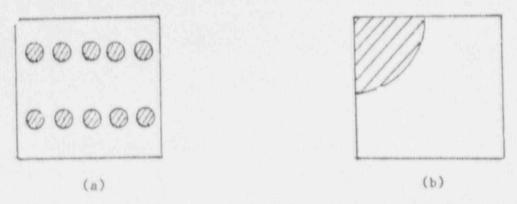


Fig. 18. Modeling (a) multiple structures or (b) fraction of a structure as one thermal structure

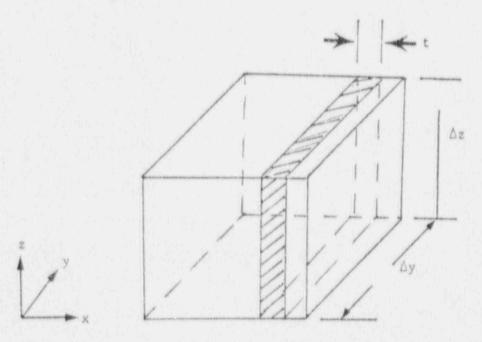


Fig. 19. Slab structure element

structure with surface area equal to 10 times the surface area of one pin. Similarly, as shown in Fig. 18b, we can consider a fraction of a pin also as a thermal structure.

- · A slab structure (Fig. 19) can be considered as either
 - -A two-sided thermal structure with surface area for each side = $\Delta y \Delta z$ and thickness = t, or
 - -A one-sided thermal structure, the other side (inner surface) being adiabatic, with outer surface area = $2\Delta y\Delta z$ and thickness = t/2.
- In many cases, we find that solid structures are uniformly distributed, e.g., fuel pins in a reactor core, heat exchanger tubes, etc. For modeling of such uniformly distributed thermal structures, we have provided an alternate way for specifying heat transfer surface area. This is done through the variable

RODFR, which has different meanings depending on what and how we specify. We explain this through some illustrations:

Positive RODFR: COMMIX -1C computes heat transfer surface area using the following equation:

Cylindrical Structure:

Surface Area = $(2\pi \text{ r } \Delta \text{ Z}_i)$ RODFR

Plane Structure

Surface Area = RODFR

Spherical Structure

Surface Area = $4\pi r^2$ RODFR

Here, r is the surface radius (outer radius for outer surface or inner radius for inner surface) and Δ Z_{1} is the axial length of coolant cell. Therefore, the definition of RODFR is

RODFR: Number or fraction of rods interacting with coolant cell, for a cylindrical or spherical structure, and

RODFR = surface area

for a slab-type structure. With this definition, we specify RODFR = 10 for the illustration in Fig. 18a, and 0.25 for the illustration in Fig. 18b.

Negative RODFR: If we specify a negative value, then COMMIX uses the following relation to compute heat transfer surface area:

Cylindrical Structure

Surface Area = $(2\pi \text{ r } \Delta \text{ Z}_1|\text{RODFR}|)^{\bullet}$ (Cell area normal to structure axis)

Plane Structure

Surface Area = |RODFR| *(Cell area parallel to structure surface area)

Spherical Structure

Surface Area = $4\pi r^2$ | RODFR| *Cell Volume

Therefore, the definition of RODFR for negative specification is

OF

or

$$|RODFR| = \frac{number of spheres}{cell volume}$$

With this definition, we specify

$$RODFR = -2/ab$$

for the cell at the upper left corner in Fig. 20.

RODFR =
$$-\frac{1}{2\pi r_{m}(r_{2} - r_{1})}$$

= $-\frac{1}{\pi(r_{1} + r_{2})(r_{2} - r_{1})}$

for the illustration in Fig. 21, and

$$RODFR = -1$$

for the illustration in Fig. 19.

5.5 Input Preparation

5.5.1 Introduction

There are four sections of COMMIX input where we specify information that is directly related to thermal structure:

- NAMELIST/GEOM/.
- · NAMELIST/DATA/.
- · Thermal-Structure Prototype Records.
- · Thermal-Structure Location Records.

In addition to these directly related inputs (which are described in the following sections), we must supply material properties and heat transfer correlations (described in Sec. 8).

5.5.2 NAMELIST-Input

- NAMELIST/GEOM/: Here, we input the variable ISTRUC=1, which indicates
 that thermal-structure-related input is to be read and a computation is to be
 performed.
- NAMELIST/DATA/: Here, the TS-related variable is NEWTS. We specify NEWTS=1 only if we want to
 - -Modify or update thermal-structure-related information using the restart option, or
 - -Input new thermal-structure-related information

at the start of either a steady-state run (ISTATE=0) or a transient run (ISTATE=2). This variable comes into operation only with ISTRUC=1 and ISTATE=0 or 2.

	(1		1.50	
b	0	0	0	0	0
	0	0	0	0	0
2 b	0	0	0	0	0
	0	0	0	0	0
36	0	0	0	0	0
	0	0	0	0	0

Fig. 20. Uniformly distributed rod bundles in a nonuniform grid

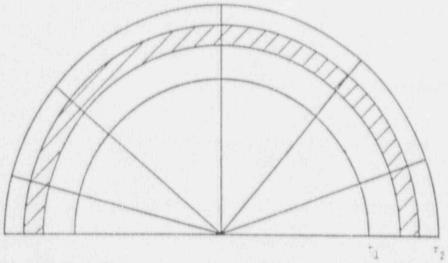


Fig. 21. Cylindrical shell with nonuniform azimuthal grid

5.5.3 Prototype Records

The thermal structure prototype records are the input records where we input all geometric and physical information for all thermal structures. A detailed description of this input is given in Appendix A. We describe it briefly here to explain some input-related rules.

- For each TS we have a set of input records.
- Each set contains several NAMELIST records. They are to be in the following order:
 - &T For information related to thermal structure.
 - &F For information related to outer surface fluid.

- &M For information related to Material 1 and Gap 1
- &M For information related to Material 2 and Gap 2

.

(Include one NAMELIST/M/ for each material region in a thermal structure.)

- &F For information related to inner-surface fluid. This record is included only if the TS is two-sided. If the inner surface is adiabatic or a symmetry boundary, this record is not required.
- The numbering of material regions begins as we traverse from outer surface to inner surface. To illustrate the ordering system, two examples are presented.

Example 1: Ordering sequence of records for TS shown in Fig. 22a:

&T N=, IXYZ=, NT=, RODFR=, OUTR=, &END

&F IHT=, &END

&M MI=, NP=, DR=, Q=, SGAP=, HGAP=, &END

&M MI=, NP=, DR=, Q=, SGAP=, HGAP=, &END

&F IHT=, &END

Example 2: Ordering sequence of records for TS shown in Fig. 22b:

&T N=, IXYZ=, NT=, RODFR=, OUTR=, &END

&F IHT=, &END

&M MI=, NP=, DR=, Q=, SGAP=, HGAP=, &END

&M MI=, NP=, DR=, Q=, SGAP=, HGAP=, &END

&M MI=, NP=, DR=, Q=, SGAP=, HGAP=, &END

&M MI=, NP=, DR=, Q=, SGAP=, HCAP=, &END

The meanings of all FORTRAN variables referred to in the TS prototype records are given in Table 9.

Note: If a fluid or a adiabatic surface follows a material, the gap properties are ignored. The gap properties are used for a given material only when another material follows.

Note: If there is no gap between two materials, we specify a high heat transfer coefficient, e.g.,

SGAP = 0.0, HGAP = 1.E30.

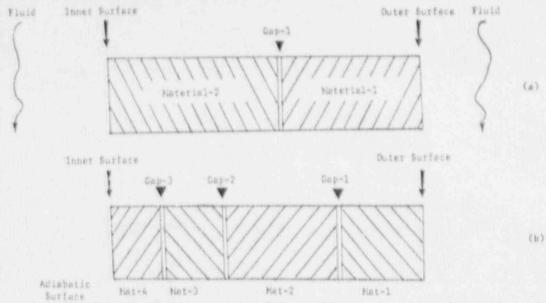


Fig. 22. Numbering system of thermal-structure material regions

Table 9. FORTRAN variables for TS prototype records

Variable	Description				
N	TS#				
IXYZ	Number to describe shape and axis alignment (see Appendix A for numbers				
NT	Transient function number for heat sources				
RODFR	Rod fraction to specify surface area				
OUTR	Outer-surface radius (m)				
IHT	Heat-transfer correlation number				
MI	Material number (see Sec. 8)				
NP	Number of grid partitions in the material for finite-difference analysis				
DR	Thickness of each partition (m)				
8	Volumetric heat source (W/m³)				
SGAP	Gap thickness (m)				
HGAP	Gap heat transfer coefficient (W/m2°C)				

5.5.4 Location Records

The purpose of the location records is to input TS-element location information. The format of specifying location information is very similar to that of boundary value and internal cell initialization records. The FORMAT is (A4, 714):

	OUT	N	IB	110	JB	JE	KB	KE
or								
	IN	N	IB	IE	JB	JE	KB	KE

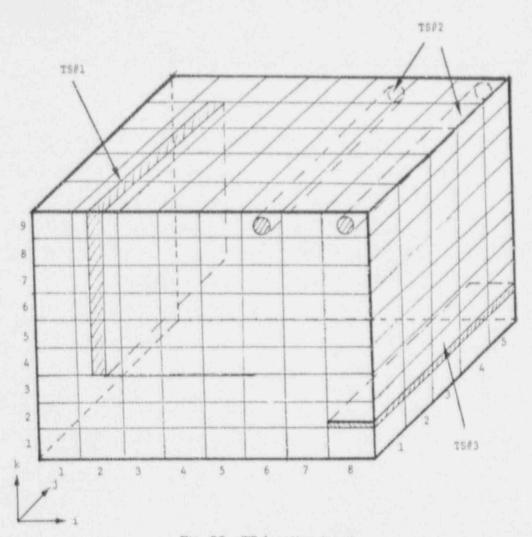


Fig. 23. TS location input

For a two-sided structure, we specify OUT to describe the locations of the outer-surface cells and IN to describe the locations of the inner-surface cells. For one-sided structures, we have either "IN" or "OUT" records only. The variable N stands for TS number and IB ... KE stands for the beginning and ending of i, j, and k indices.

For easy understanding of location input records, we illustrate a simple geometry, as shown in Fig. 23. The input for the thermal structures in Fig. 23 will be as follows:

OUT 1 2 2 1 4 4 9
OUT 2 8 8 1 5 9 9
OUT 2 6 6 1 5 9 9
OUT 3 8 8 1 5 2 2
IN 3 8 8 1 5 1 1

6 Force-Structure Modeling

6.1 Introduction

The purpose of force-structure modeling in COMMIX-1C is to permit consideration of frictional resistance due to irregular geometry and the presence of solid structures in ϵ flow domain. In COMMIX-1C, we account for this effect by providing an additional distributed-resistance source term in the momentum equation. To include this distributed-resistance source term in computation, we must provide the required information.

6.2 Resistance Correlation

In the literature, pressure drop due to obstructions is expressed in many different forms, e.g.,

$$\Delta p = 4 \frac{L}{D} \frac{1}{2} \rho v^2 f$$
, (6.1a)

$$= \frac{L}{D} \frac{1}{2} \rho v^2 C_D. \tag{6.1b}$$

$$=\frac{1}{2}\rho v^2 K$$
 (6.1c)

The coefficients f, CD, K, etc. have been given different names, e.g., Fanning friction factor. Darcy friction factor, drag coefficient, loss coefficient, etc., depending on the form of the equation.

In COMMIX-1C, we use the following general forms:

$$\Delta p = C_1 \frac{L}{D} \rho v^2 f . \qquad (6.2)$$

In terms of a distributed-resistance R, Eq. 6.2 is

$$R = C_1 \rho \frac{\text{vivi}}{D} f = \frac{\Delta p}{L}. \tag{6.3}$$

Here, $L[\Delta x (\Delta r), \Delta y (r\Delta \theta), \text{ or } \Delta z]$ is the cell length of a momentum control volume, D is the hydraulic diameter or characteristic length, and C_1 is the coefficient to account for different definitions of friction factor f.

The friction factor f in Eqs. 6.2 and 6.3 is generally a function of Reynolds number. In COMMIX-1C, we use the following form to express the friction factor correlation:

$$f = a_{\ell} Re^{b_{\ell}} + c_{\ell} \tag{6.4a}$$

for laminar flow when the Reynolds number Re (= $\rho u d/\mu$) is less than a predefined transition Reynolds number Re_{tr}, and

$$f = a_t Re^{b_t} + c_t ag{6.4b}$$

for turbulent flow (Re > Re $_{tr}$). The subscripts ℓ , t, and tr stand for laminar, turbulent, and transition, respectively.

6.3 Input Requirements

We can see from the form of the equations in the preceding section that we need the following inputs:

- Variables C₁ (FORCEF) and D(CLENTH) to compute resistance-source term (Eq. 6.2).
- Variables at (ACORRL),, ct(CCORRT), and Retr (REYTRN) to compute the friction factor f (Eq. 6.4), and
- · Reference length d (REYLEN) for Reynolds number Re.

In addition, we have added the following input requirements:

- · NEWFOR A signal to inform that new force-structure input must be read.
- · NFORCE Number of force structures.
- · NCORR Number of friction factor correlations.
- ICORR
 Linkage between a force structure and correlation number, e.g.,
 ICORR(3)=4 means that correlation 4 is to be used for force structure 3.
- · Force-structure locations.

All input variables related to force structure are listed in Table 10.

6.4 Force-Structure Locations

The force-structure location information is provided through force-structure specification records. The FORMAT is (A4, 714):

We specify XFOR, YFOR, or ZFOR to input the direction of force. The variable NF stands for the force-structure number, and IB ... KE stand for beginning and ending i, j, k indices of cell locations. For more details relating to force-structure location input, see Appendix A.

Table 10. Input variables related to force-structure modeling

FORTRAN Name ^a	Description of Variable	COMMIX Input Section	Remarks
NFORCE	No. of force structures	NAMELIST/GEOM/	
NEWFOR	Signal for new force-structure input	NAMELIST/DATA/	= 0 for no. = 1 for yes; applicable for ISTATE = 0 or ISTATE=2
CLENTH(NF)	D (Eq. 6.2)	NAMELIST/DATA/	Given a negative value if desired to use Eq. 6.1c; i.e., when L = D
FORCEF(NF)	C ₁ (Eq. 6.2)	NAMELIST/DATA/	
NCORR	No. of correlations	NAMELIST/DATA/	
ICORR(NF)	Correlation linkage	NAMELIST/DATA/	See Sec. 6.3
ACORRL(N)	a/ (Eq. 6.4a)	NAMELIST/DATA/	
BCORRL(NC)	b _ℓ (Eq. 6.4a)	NAMELIST/DATA/	
CCORRL(NC)	c/ (Eq. 6.4a)	NAMELIST/DATA/	
ACORRT(NC)	at (Eq. 6.4b)	NAMELIST/DATA/	
BCORRT(NC)	b ₁ (Eq. 6.4b)	NAMELIST/DATA/	
CCORRT(NC)	ct (Eq. 6.4b)	NAMELIST/DATA/	
REYTRN(NC)	Retr	NAMELIST/DATA/	Reynolds no. for laminar/ turbulent transition
REYLEN	d	NAMELIST/DATA/	Reference length for Reynolds no.
XFOR YFOR ZFOR	Force-structure location	Force-structure specification records	For direction and location, see Sec. 6.4

aNF is a force-structure number: NC is a correlation number.

6.5 Modeling Recommendations

6.5.1 Staggered Grid System

In the finite-volume formulation, frictional resistance due to a solid structure in a flow domain is considered an additional source term in the momentum equation. Because a staggered-grid system is used in COMMIX-1C, the control volumes for the momentum equations are displaced, as illustrated in Fig. 24. It is therefore important to remember during modeling of the resistance term that:

- The distributed-resistance source term is for the staggered control volume as shown in Fig. 24, and
- * The reference velocity used in the resistance source term equation is the velocity at the face of a cell.

To illustrate this point, we consider the case of a sudden enlargement, as shown in Fig. 25. The pressure loss due to abrupt change in area is generally expressed in terms of the loss coefficient K_1 or K_2 , depending upon which reference velocity is used:

$$\Delta p = K_1 \frac{1}{2} \rho V_1^2 ,$$

$$= K_2 \frac{1}{2} \rho V_2^2 ,$$

where subscripts 1 and 2 refer to smaller and larger cross-sections, respectively. In such cases, the user must look at the location of abrupt expansion (see Fig. 25) and then prescribe a suitable correlation for either K_1 or K_2 .

6.5.2 Friction-Factor Library

Occasionally, the COMMIX-1C user may find that the desired correlation is not of a form described in Sec. 6.2. The user is then faced with two choices:

- · Approximate the correlation to fit the input form, or
- · Use the friction-factor library.

The friction-factor library has been created to accommodate up to 50 different additional correlations corresponding to values of ICORR(NF) from 50 to 99. Currently, only seven correlations, as described in Volume I, have been added to the library.

The user who wishes to define an additional correlation can first examine the subroutine FORCES to see what correlation numbers are free and available. Then, with other library correlations as a guide, a new correlation can be inserted appropriately in subroutine FORCES and recompiled.

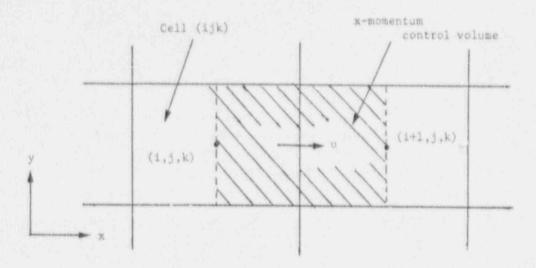
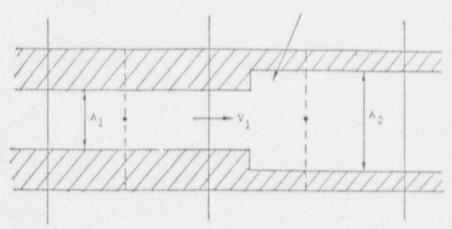


Fig. 24. x-Momentum control volume in a staggered grid system

Momentum Control Volume



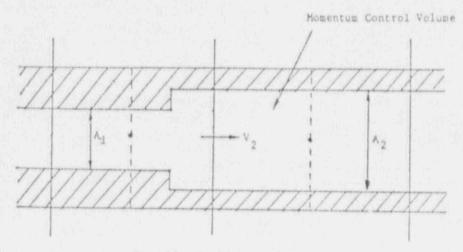


Fig. 25. Sudden enlargement

6.5.3 List of Correlations

To save the user time in searching the vast literature, we have collected a set of correlations that we feel are most commonly needed by COMMIX-1C users. These correlations are listed in Appendix C.

We caution here that the correlations in Appendix C are not necessarily the only and best relations. We welcome feedback and comments from all users so that we can add other correlations and update the existing relations.

7 Solution Procedure

7.1 Introduction

As described in Volume I, COMMIX-1C employs the implicitness parameter α in the formulation of the general finite-difference equations. Also available in COMMIX-1C are the three matrix solvers for the scalar transport equations and the pressure equation. These options make numerical computation more efficient for a given problem. In this section, we will describe how to use these options and provide some guidance on selecting the proper method for a given application. The convergence and relaxation parameters are also described in this section.

7.2 Solution Methods

A list of the variables related to the solution procedure is given in Table 11. The implicit parameter α is represented by the FORTRAN name ALPHA and is in input section of NAMELIST/DATA/. The fully implicit scheme is recommended and, by default, ALPHA = 1.0. For the vast majority of simulations, the fully implicit scheme should be used because it does not have the time-step restriction. For very fast transient, the semi-implicit scheme may be preferred. Any value of α other than 1 is not recommended at this time because not enough testing has been performed. Finally, a word of caution on the use of the semi-implicit (α = 0) solution procedure. The operational experience of COMMIX-1C has been primarily with the fully implicit solution scheme (α = 1). This is particularly true for the auxiliary models such as the k- ϵ two-equation turbulence model, the flow-modulated skew-upwind difference scheme, etc., where almost all experience has been with the fully implicit solution procedure. Therefore, use of these auxiliary models is recommended only with the fully implicit solution procedure.

The user can choose one of the matrix solvers for the scalar transport equations (energy, k, and e) and the pressure equation. The successive overrelaxation (SOR) method and the Yale Sparse Matrix Package (YSMP) are suitable for both the symmetric and non-symmetric matrix and therefore can be selected to solve both the scalar transport equations and the pressure equation. The preconditioned conjugate gradient (PCG) method is applicable for symmetric matrix and is therefore suitable for the pressure equation only. The FORTRAN name ISOLVE is the flag used to choose the matrix solver for the scalar transport equations. If ISOLVE = 0, SOR is selected, and if ISOLVE = 1, YSMP is selected. The FORTRAN name ISOLVR is the flag for choosing the matrix solver for the pressure

Table 11. Variables related to solution procedure

FORTRAN Name	Description	COMMIX Input Section	Remarks
ALPHA	Implicitness parameter	NAMELIST/DATA/	= 0.0 for semi-implicit = 1.0 for fully implicit
ISOLVE	Flag to choose matrix solver for scalar transport equations (energy, k, and ε)	NAMELIST/GEOM	= 0 for SORa = 1 for YSMPb
ISOLVR	Flag to choose matrix solver for the pressure equation	NAMELIST/GEOM/	= 0 for SOR = 1 for YSMP = 11 for PCG ^c

aSOR: successive overrelaxation method.

bYSMP: Yale Sparse Matrix Package.

cPCG: Preconditioned conjugate gradient method.

equation. ISOLVR = 0, 1, and 11 corresponds to the matrix solver of SOR, YSMP, and PCG, respectively. If SOR is selected, the user should specify the convergence parameter ϵ_1 and the relaxation parameter omega (which we describe in the next section). If the YSMP is selected, the user should input the parameters NNZERO and NSPACE in the NAMELIST/GEOM/. The values of these two parameters are not known beforehand. The best way is to input some arbitrary values for NNZERO and NSPACE, and submit a job. Then the output will indicate the proper values to use for both NNZERO and NSPACE. This procedure may have to be repeated several times.

As a rough guide, YSMP is most efficient if the number of computational cells is less than 1000. If the number of computational cells is greater than 2000, then the SOR method should be selected for the scalar transport equations and the PCG method for the pressure equation. If the number of computational cells is between 1000 and 2000, there is no clear advantage in one method over the others and the choice is problem-dependent.

Finally, it should be noted that the user can choose to skip the calculation of either the momentum equations or the energy equation. For example, if one wishes to perform calculations for an isothermal flow, the parameter IFENER should be set equal to zero and the energy equation is bypassed during the solution sequence. Similarly, if the user wishes to omit calculations of the momentum equations, the parameter IFMOM should be set equal to zero and the momentum equations are bypassed during the solution sequence.

7.3 Convergence Parameters

There are a number of convergence criteria employed in COMMIX-1C (Table 25 in Volume I). The user must input these convergence parameters for the iterative solution schemes such as the successive overrelaxation method and the preconditioned conjugate

gradient method. Table 12 lists all of the convergence parameters required as input and the default value for each parameter. All of the convergence parameters should be in the NAMELIST/DATA/ section of the input.

7.4 Relaxation Parameters

The finite-volume discretization equations in COMMIX-1C have been constructed so that if there were no interlinkages and nonlinearities, convergence would be certain. However, because the equations of interest almost always contain nonlinear and interlinked influences, care should be taken to prevent divergence. One simple strategy is to slow the changes that would occur from iteration to iteration. This is accomplished with under-relaxation.

7.4.1 Implicit Underrelaxation

The general finite-volume discretization equation of COMMIX is

$$a_0^{\bullet} \phi_0 = \sum_{\ell} a_{\ell}^{\bullet} \phi_{\ell} + b_0^{\bullet}$$
 (7.1)

where the subscript & denotes the neighbor points. This equation can be modified as follows: from Eq. 7.1, we can write

$$\phi_0 = \sum_{\ell} \frac{a_{\ell}^*}{a_0^*} \phi_{\ell} + \frac{b_0^*}{a_0^*} \ . \tag{7.2}$$

Also, let

$$\phi_0^{\text{new}} = \omega \phi_0 + (1 - \omega)\phi_0^*$$
, (7.3)

where ϕ_0^* denotes the last iteration value of ϕ_0 , ϕ_0 denotes the value obtained directly if Eq. 7.1 is solved, and ω is the underrelaxation factor. Substitution of Eq. 7.2 in Eq. 7.3 and after rearrangement gives

$$\left(a_0^{\bullet}/\omega\right)\!\phi_0^{\text{new}} = \sum_{\ell} a_{\ell}^{\bullet}\phi_{\ell} + b_0^{\bullet} + (1-\omega)\!\left(a_0^{\bullet}/\omega\right)\!\phi_0^{\bullet} \ . \tag{7.4}$$

When ϕ_0 becomes equal to ϕ_0 (i.e., the iterations converge). Eq. 7.4 becomes identical to Eq. 7.1. In the meantime, however, Eq. 7.4 would have a tendency to keep the resulting ϕ_0^{new} closer to ϕ_0^{than} would Eq. 7.1, provided the relaxation factor ω is less than 1. A value of ω close to zero would indicate very heavy underrelaxation.

For the velocity components, a conservative value of ω = 0.8 can be used. The energy equation can be conservatively underrelaxed by using ω = 0.8. These values should be regarded only as initial suggestions; a proper set of ω values should be obtained by actual experience with a given class of problems. In COMMIX-1C, the input parameters OMEGAV, OMEGAE, OMEGAK, and OMEGAD are provided for implicit underrelaxing velocities u, v, and w, enthalpy h, turbulence kinetic energy k, and dissipation rate of turbulence kinetic energy k, respectively. Table 13 lists all underrelaxation parameters and default values employed in COMMIX-1C. As shown in Table 13, two additional underrelaxation

Table 12. Convergence parameters

FORTRAN Name	Symbol	Description	Default Value
EPS1	ε	Mass convergence for pressure equations	10-4
EPS2	ε2	Mass convergence for pressure equations	10-6
EPS3	£3	All transport variables (h. k. e. u. v. and w)	5 x 10 ⁻⁵
EPS5	€5	Enthalpy	10-5
EPS6	€6	Turbulence parameters k and s	10-5

Table 13. Underrelaxation parameters and default values employed in COMMIX-1C

FORTRAN Name	Default Value	Remarks
OMEGAV	0.8	
OMEGAE	0.8	Velocity components
OMEGAK		Enthalpy
	0.7	Turbulence kinetic energy
OMEGAD	0.7	Rate of dissipation of turbulence kinetic energy
OMEGAR	1.0	Density
OMEGAT	1.0	Turbulent viscosity

Table 14. Relaxation parameters for SOR method, und default values, employed in COMMIX-1C

FORTRAN Name	Default Value	Remarks	
OMEGA	1.5	Pressure	
RELAXE	0.95	Enthalpy	
RELAXK	0.8	Turbulence kinetic energy	

parameters. OMEGAR for density and OMEGAT for turbulent viscosity, are available in COMMIX-1C. The default value for these two parameters is 1.0.

7.4.2 Successive Overrelaxation

Table 14 is a list of the relaxation parameters required for using the successive overrelaxation (SOR) method and the default values for these parameters.

8 Auxiliary Input

In addition to geometry specification, initialization, and model input, the user may have to provide several auxiliary inputs. These inputs are briefly described here; more-detailed information is presented in Appendix A.

8.1 Heat Transfer Correlation

The purpose of the heat transfer correlation input is to provide information required in the calculation of the surface heat transfer coefficient in thermal-structure models. Currently, there are two types of heat transfer correlations available in COMMIX-1C. The linkage of the heat transfer coefficient to the thermal-structure model is through the variable IHT in the thermal-structure prototype records NAMELIST/F/. There are three input parameters associated with a particular IHT:

- · IHTCOR(IHT) Heat transfer correlation number.
- · HTCLEN(IHT) Characteristic length, and
- HTCMUL(IHT) Heat transfer coefficient multiplier.

For example, if IHT = 2, and

IHTCOR(2) = 8.

HTCLEN(2) = 2.0

HTCMUL(2) = 3.0.

this represents that heat transfer correlation number 8 will be used for this particular thermal structure, the characteristic length used in the calculation of the Reynolds number and Nusselt number is 2.0 meters, and the calculated heat transfer coefficient will be multiplied by a factor of three.

The two types of heat transfer correlation in COMMIX are:

1 If IHTCOR = 1 - 10:

$$h = h_0 \times Nu \times k/d \tag{8.1}$$

where
$$h_0$$
 = heat transfer coefficient multiplier (HTCMUL),
 $Nu = C_1 + C_2 Re^{C_3} Pr^{C_4}$, (8.2)

Re = Reynolds number,

Pr = Prandtl number.

k = thermal conductivity, and

d = characteristic length (HTCLEN)

2. If IHTCOR = 11 - 20:

$$h = h_0 (C_1 + C_2 Re^{C_3} Pr^{C_4})$$
(8.3)

The constants C_1 , C_2 , C_3 , and C_4 are user input coefficients, and the FORTRAN names for these coefficients are HEATC1, HEATC2, HEATC3, and HEATC4, respectively. All input parameters for the heat transfer coefficient calculations should be in the section of NAMELIST/DATA/.

The user can also add other heat transfer correlations if the correlations given by Eqs. 8.1 and 8.3 are not appropriate. The new addition can be defined by using an IHTCOR number greater than 20. The new correlation should be inserted in subroutine HTCOEF and recompiled.

8.2 Fluid and Material Properties

Fluid properties are determined by the variable MATYPE in the input section of NAMELIST/DATA/. The values of MATYPE may be any integer from 1 to 24. When the value of MATYPE is from 1 to 20, the fluid properties are computed from the simplified equations. If MATYPE is between 21 and 24, the fluid properties are calculated by rigorous subroutines for the following fluids:

- 21 water liquid,
- 22 water vapor.
- 23 sodium liquid.
- 24 sodium vapor.

The simplified equations for fluid and material properties enthalpy h, density $\rho,$ thermal conductivity $\lambda,$ and viscosity μ are

$$h\left(\frac{J}{kg}\right) = C_0^h + C_1^h T + C_2^h T^2 + C_3^h P , \qquad (8.4)$$

$$\rho\left(\frac{kg}{m^3}\right) = C_0^\rho + C_1^\rho T + C_2^\rho P / (T + 273.16) , \qquad (8.5)$$

$$\lambda \left(\frac{W}{m - {}^{\circ}C} \right) = C_0^{\lambda} + C_1^{\lambda} T + C_2^{\lambda} T^2 , \qquad (8.6)$$

$$\mu(Pa * s) = C_0^{\mu} + C_1^{\mu} T + C_2^{\mu} / (T + 273.16), \qquad (8.7)$$

where T is in $^{\circ}$ C and P is in Pa. For each property, the user must input the constants C_0 , C_1 , etc. The FORTRAN names for these constants are

CØH, C1H, C2H, C3H CØRO, C1RO, C2RØ Coefficients of enthalpy equation, Coefficients of density equation, CØK, C¹K, C2K CØMU, C1MU, C2MU Coefficients of conductivity equation, and Coefficients of viscosity equation

The linkage of the material properties to the thermal structure model is through the variable MI in the thermal structure prototype records NAMELIST/M/. For example, if MI = 2 for a given material and

CØK = 20., 40., 60.,

CIK = 10-3, 10-4, 10-5,

this means that the thermal conductivity of this material is given by

 $\lambda = 40 + 10^{-4} \times T$.

Similarly, if MATYPE - 1, the fluid properties are calculated by

 $\lambda = 20 + 10^{-3} \text{ T}.$

8.3 Turbulence Modeling

In COMMIX-1C, two options are provided to account for the effect of turbulent flows:

- · Constant-diffusivity model, and
- k-ε two-equation turbulence model.

The theory and equations relating to these models are described in Volume I. Here, we present only the information needed by the user.

8.3.1 Signal Parameter

The variable ITURKE in NAMELIST/GEOM/ specifies which turbulence model is to be used:

ITURKE = 0 No turbulence model (laminar flow) or constant-diffusivity model.

12 k-ε two-equation turbulence model.

8.3.2 Constant-Diffusivity Model

In the constant-diffusivity model (ITURKE = 0), a user must specify the values of turbulent viscosity (μ_{tur}) and turbulent conductivity (λ_{tur}) in NAMELIST/DATA/. The corresponding FORTRAN variables are TURBV and TURBC, respectively.

It is recommended that values being prescribed have been obtained from experimental data. If such values are not available, a user can provide his/her own estimate or use the procedure suggested in Sec. 6.2 of Volume I to estimate these parameters.

8.3.3 k-E Two-Equation Turbulence Model

In the two-equation model (ITURKE = 12), we solve the transport equations of turbulence kinetic energy ϵ and dissipation rate of turbulence kinetic energy ϵ . As described in Volume I, there are a total of eight constant coefficients employed in the k- ϵ two-equation turbulence model. Table 15 is a list of the FORTRAN names and default values of these coefficients. These parameters are required only if the user wishes to use values different from the default values given in Table 15. These parameters should be in the input section of NAMELIST/DATA/.

In addition to the inputs described previously, there are several inputs that the user may need for the k-ɛ two-equation turbulence model (see Table 16). Most of these parameters were already described in previous sections. For example, the relaxation parameters are described in Sec. 7.4 and the boundary turbulence parameters (TKB and TDB) are described in Sec. 4.2. They are presented here mainly for cross-reference because these parameters fit in both classifications.

All parameters in Table 16, with the exception of TKB and TDB, should be in the input section of NAMELIST/DATA/. TKB and TDB should be in the surface-element initialization records.

8.4 Numerical Diffusion

When flow is inclined to grid lines, and the pure-upwind scheme is used to formulate convection terms. Sumerical Assistant may result. To reduce numerical diffusion, we have provided an additional option in COMMIX-1C, the flow-modulated skew-upwind discretization scheme. To use this option, a user needs to input only one variable (ISKEW) in the NAMELIST/DATA/. If ISKEW = 0 (default), the pure-upwind difference scheme is used. If ISKEW = 2, the flow-modulated skew-upwind difference scheme will be activated.

8.5 Time-Step Size

COMMIX performs thermal-hydraulic calculations by marching in time. The values of the dependent variables at a given time t and time-step n are known. The values of the dependent variables at time $t+\Delta t$ and time-step n+1 are calculated. By repeating this procedure, the thermal-hydraulic conditions are determined for $\frac{1}{2}$ desired time span.

For a steady-state calculation, the same procedure is followed. We start with an initial state and continue the marching-in-time process until the values of all dependent variables become slowly varying. The time step size for the implicit-steady-state calculation can be very large, e.g., as much as 10-20 times the Courant time-step criterion.

In COMMIX, there are two options for selecting the time-step size:

- The user can prescribe the desired time step size as inp.: details of this
 input are given in Appendix A.
- · The automatic time-step option can be used.

Table 15. Coefficients employed in k-ɛ twoequation turbulence model

FORTRAN Name	Symbols Used in Volume I	Default Value
PRNDLH	σh	0.9
PRNDLK	$\sigma_{\mathbf{k}}$	1.0
PRNDLD	σι	1.3
CT1	C ₁	1.44
CT2	C ₂	1.92
CDTURB	CD	0.09
AKAPPA	K	0.42
EE	E	9.0

Table 16. Possible additional input for k- ϵ two-equation turbulence model

ariable Function		Default Value
ITMAXK	Maximum number of iterations for k equation	29
OMEGAT	Relaxation factor for turbulent viscosity	
OMEGAK	Relaxation factor used in the solution of k equation	0.7
OMEGAD	Relaxation factor used in the solution of ϵ equation	0.7
RELAXK	Relaxation factor for k	0.8
EPS6	Convergence criterion for the k and ϵ equations	10-5
ТКВ	Boundary turbulence kinetic energy	10-16
TOB	Dissipation rate of boundary turbulence kinetic energy	10-10

In the automatic time-step option, the time-step size is evaluated on the basis of the Courant condition:

$$\Delta t = C_1 \, \Delta t_C, \tag{8.8}$$

where C_1 is the user-prescribed coefficient and Δt_c is the time-step size evaluated from the Courant condition. The Courant time step-size is the minimum time required for fluid to be convected through a cell. It is to be noted that the automatic time-step option

described here is not an optimum time-step size for a given transient condition. Additional work is needed to develop an automatic time-step selection scheme as described in Vol. I, where an optimum time-step size is selected during the course of a transient calculation.

The following input variables are related to time-step size:

IDTIME	Signals whether user-specified or Courant time-step.
DT(1) DT(2) LASTDT	DT(1) is the time-step size for steps 1 through LASTDT. DT(2) is the time-step size for steps after LASTDT.
TIME	Factor C1 used for multiplying the Courant time step size
	(Eq. 8.8).

There are several other time-related parameters (see Table 17). These parameters provide the user with additional flexibility in controlling how a particular run should be conducted. For example, if the user wants to run for just one time-step (for debugging), the parameter NTMAX should be set equal to 1. If the user wants to run a particular problem for just one minute, the parameter TIMAX should be set equal to 60.

8.6 Output

An input procedure, described in Appendix A, is provided for printing array values of a range of variables at given locations (specified plane) and at a given time or time step.

3 Steady-State Calculation

9.1 Introduction

In COMMIX, even when analyzing a transient problem, we must first obtain a steadystate solution to generate an initial condition for the transient problem.

To perform a steady-state calculation, we consider the problem as if it were a transient problem. We prescribe an estimated distribution of dependent variables as our initial condition and continue marching in time until the distribution becomes slowly varying and satisfies the prescribed convergence criteria.

9.2 Input Preparation

To start a steady-state calculation, we prescribe:

- · Control flag ISTATE = 0.
- · Control flag IFRES = 1.
- ALPHA = 1; for steady-state simulation, we recommend the fully implicit procedure.
- · Geometrical information.

Table 17. Time-related parameters

Name	Description	Default Value
NTMAX	Maximum time-step for a given run	99999
TIMAX	Maximum time for a given run	3.6 x 10
ITEMER	 = 0, no subroutine time information shown = 1, subroutine time information shown at the end of a run = 2, subroutine time information shown after every call 	0
TREST	If the elapsed run time exceeds TREST, the run is terminated after optionally writing a restart file	3600
TSTART	This value should be reset to zero at the beginning of a transient run (STATE=2)	0.0

- Constant-value boundary conditions (use the surface-element initialization records if the boundary conditions are nonuniform).
- Our best estimated values as initial condition; to save computer running time, it is recommended that initial estimated values be prescribed as closely as possible to the expected solution.
- Number of iterations IT = 1. Because we are performing a steady-state simulation, each time-step represents a steady-state iteration; therefore, more iterations per time-step are not required.
- Time-step size DT can be large. We recommend starting with DT = 1000 s or larger. If this causes a convergence problem, it then can be reduced to, say, 100 s or 10 s or even less.
- · Fluid and material properties.
- · Other ancillary information, e.g., output printing desired.
- · Force-structure input, if any.
- Thermal-structure modeling with heat source, if any. NOTE: For a steadystate calculation, only the thermal structures with heat sources need to be considered.
- · Turbulence model input, if necessary.
- · Flow-modulated skew-upwind discretization scheme input, if necessary.

The control flag IFRES = 1 implies that we are starting a new case and that at the end of the run we want the results to be written on a restart file. If we do not desire a restart file to be written, we prescribe IFRES = 0. For continuation of a steady-state run, we specify

- · ISTATE = 1 and
- IFRES = 3

in the continuation run input.

9.3 Steady-State Convergence Criteria

We define a steady-state solution as having been achieved when the following steadystate criteria are satisfied simultaneously:

$$\begin{split} & \left(\frac{|\Delta h|}{h}\right)_{max} < \epsilon_3 \;, \\ & \left(\frac{|\Delta u|}{VELMAX}\right)_{max} < \epsilon_3 \;, \\ & \left(\frac{|\Delta v|}{VELMAX}\right)_{max} < \epsilon_3 \;, \\ & \left(\frac{|\Delta w|}{VELMAX}\right)_{max} < \epsilon_3 \;, \text{ and} \\ & \left(\frac{|\delta w|}{VELMAX}\right)_{max} < DCONV \;. \end{split}$$

Here Δu , ..., Δh are the changes between successive time steps, δ is the mass residue, ϵ_3 is the steady-state convergence criterion, VELMAX is the maximum of all velocity magnitudes, and DCONV is the mass convergence parameter calculated using the relation

$$DCONV = \varepsilon_1 \left[\left(\frac{\rho \gamma_1 u_1}{\gamma_v \Delta x_1} \right)_{max} + \varepsilon_2 \right] , \qquad (9.1)$$

where ϵ_1 and ϵ_2 are the input convergence constants, subscript i stands for the three coordinates, γ_1 is the suface porosity, and γ_2 is the volume porosity. The default values for ϵ_1 , ϵ_2 , and ϵ_3 are 10^{-4} , 10^{-6} , and 5×10^{-5} , respectively.

10 Transient Calculations

10.1 Introduction

We consider that in COMMIX any one or a combination of the following conditions can make a problem transient:

- · Transient velocity boundary condition.
- · Transient temperature and surface heat flux boundary conditions,

- · Transient pressure boundary condition, and/or
- · Transient heat source.

10.2 Procedure

For running a transient problem, we recommend the following procedure:

- Obtain a steady-state solution using constant-value boundary conditions and guessed initial distributions, and write the results on a restart file. The constant values to be used for specifying the boundary conditions must be the values at time t = 0 of the transient problem.
- Run the transient problem, using the restart data and the following additional input in NAMELIST/DATA/.

-ISTATE = 2.

- -TSTART = starting time of the transient.
- -KFLOW(N) = 100 + NF; this is for the transient velocity boundary cond 'on.

 NF defines the transient function number to be used for the transient condition on surface N.
- -KTEMP(N) = 100 + NF or 300 + NF; this is for the transient temperature or heat flux boundary condition. NF defines the transient function number to be used for transient condition on surface N.
- -KPRES(N) = 100 + NF; this is for the transient pressure boundary condition. NF defines the transient function number to be used for transient condition on surface N.
- -NOFQT: This is the number of the transient function that is used as a multiplier of the specified volumetric heat source (QSOU) distribution. For example, if NOFQT = 2.

 $Q(x, y, z, t) = f_2(t) \times QSOU(x, y, z).$

where Q(x, y, z, t) is the transient volumetric heat source, f_2 is the transient function number 2, and QSOU(x, y, z) is the spatial heat source distribution in the fluid.

- -TVAL: Values of the independent variable (time) of the transient functions.
- -FVAL: Values of the dependent variable of the transient functions.
- -NEND(N): Number of points used to prescribe the transient function number N.
- -Other ancillary information time step size, output, etc.

10.3 Transient Functions

In COMMIX, we use the relation

$$F(t) = F(0) * f(t)$$
 (10.1)

to prescribe the desired variation of a function with time. Here, F(0) is the value of a function at time t = 0 and f(t) is the transient function. The following information is useful relative to transient functions in COMMIX:

- A set of f and t values must be prescribed for each transient function. Cubic spline-fit coefficients are evaluated to approximate a transient function as a polynomial.
- · Up to 25 functions consisting of up to 100 points can be defined.
- All transient functions should be normalized with respect to values at time t
 = 0.
- FVAL and TVAL are the FORTRAN variable names for prescribing discrete values of f and t, respectively.
- NEND(NF) is the number of discrete f and t values prescribed for transient function #NF.
- FVAL and TVAL are one-dimensional arrays; the first value of the second transient function immediately follows the last value of the first function.
 The same pattern is followed for all subsequent transient functions.
- Discontinuities in a function can be indicated by specifying the same t value twice with the same or different f values.

10.4 Decoupled Transient Calculation

In a normal transient simulation, all three (mass, momentum, and energy) coupled conservation equations are solved at every time-step. However, by decoupling the mass-momentum and energy equations, one may save some computer running time because

- At a given time-step, we are now only solving either the mass-momentum equations or the energy equation.
- · Decoupling reduces the number of iterations required per time-step.
- With decoupling, we can use a larger time-step size.

Therefore, we have provided a decoupling option that permits the solution of the

^{*} Here, decoupling means solving either the mass-momentum or the energy equation only at a given time-step.

- -Mass-momentum equation, or
- -Energy equation, or
- -Mass-momentum and energy equations

at any time-step.

The decoupling option is ideal for:

- A very long transient that might normally require prohibitively long computer running time, but that we are willing to consider as a quasitransient problem.
- · A transient with slowly varying velocity field.
- · A transient with slowly varying energy field.

The input parameters for invoking the decoupled calculation are ISETMO and ISETEN. The positive (negative) integer value of these parameters indicate the time-step frequency with which the corresponding equation is solved (or not solved), e.g.,

 When ISETMO = 1 and ISETEN = 3, the mass-momentum equations are solved at every time-step and the energy equation is solved every third timestep, as indicated in the following table:

Time-Step 1 2 3 4 5 6 7

Equations M M M M M M M M Solved E

 When ISETMO = 3 and ISETEN = -3, the mass-momentum equation is solved every third time-step and the energy equation is not solved at every third time-step. The following table describes the coupling sequence:

Time-Step 1 2 3 4 5 6 7

Equations E E M E E M E

Solved

With proper combinations of ISETMO and ISETEN, the user can set any desired order of decoupling.

The decoupling procedure can save significant computer running time. However, the user should be aware that the decoupled solution can drift from a true solution in cases where significant changes in the energy (velocity) field occur before the energy (mass-momentum) equation is once again solved. The optimum values of ISETMO, ISETEN, and the time-step size are, of course, problem-dependent and should be obtained by actual experience for a given class of problems. This option has not been used for quite some time and is therefore not recommended.

11 Operating COMMIX-1C

11.1 Load Module Creation

To ease the task of creating load modules (binary files) to fit the size of the problem being considered, we have implemented a dynamic storage allocation scheme. Space for the geometry-dependent variables is allocated in the variable S of COMMON/SPACE/. The address of each variable is computed at the beginning of each run. These addresses are then passed into subroutines where the variables are named and variably dimensioned.

11.2 Input/Output

11.2.1 Input Data File 5

The input for File 5 is described in Appendix A. The most current version of the input description is generally distributed with the code. The input contains a mixture of NAMELIST and formatted data. It is rewound to allow for multiple passes through the file. The user may wish to change the file number of the read statements if the user's system does not provide for rewinding File 5.

11.2.2 Printed Output File 6

The printed output from COMMIX is written to File 6. A 133-character line length is assumed, with column 1 being the carriage control. The input data from File 5 and summary information, depending on the problem, are always printed. But the bulk of the output is user-specified and controlled by parameters such as ISTPR, NTHPR, NTPRNT, and TPRNT, which are described in Appendix A.

11.2.3 Restart Information Files 9 and 10

The restart capabilities of COMMIX are programmed in SUBROUTINE RESTAR. Blocks of information are written to File 10, which can be read by a subsequent job from File 9 to permit continued processing from the point at which the restart file was written.

Restart files are written optionally (see IFRES in Appendix A) in any of the following three events:

- Steady state is reached.
- · The time specified for the job has elapsed.
- · A specified time or time-step has been reached.

The first event is indirectly controlled by the convergence parameters. The second and third events can be controlled by variables described in the "Resto t Option" section under NAMELIST/GEOM/ and the "Time- and Time-Step-Related Parameters" section under NAMELIST/DATA/ in Appendix A.

After the restart information has been written to File 10, several additional records are written. These records contain, in effect, a snapshot of the simulation as it existed when the restart was written. This information can then be used, by interfacing with the user's graphics programs, to obtain graphic plots, e.g., vector and isotherm.

11.2.4 Plot Tape File 76

Prior to reaching steady state, it is generally adequate to obtain plots only for points in time at which restart files are written. Once steady state has been reached and a driving transient has been turned on, however, it is often desirable to save a complete history of the flow and temperature fields. SUBROUTINE PLTAPE provides this optional capability (see NTPLOT in Appendix A). At the beginning of File 76, a group of records containing geometry and properties information is written. Then, at user-controlled time-steps, the entire velocity and temperature fields are written. This file can then be used to interface with the user's plotting routines.

11.3 COMMIX Error Detection and Diagnostics

It is generally impossible to anticipate all the possible error conditions that one might encounter while using COMMIX. However, an attempt has been made to provide information that will guide the user through abnormal terminations.

There are many places where key variables are tested for meaningful values or where certain paths of a branch statement indicate error conditions. Some of these have been coded to call SUBROUTINE ERRORS. This subroutine prints short error messages and determines whether processing can continue or must terminate.

The "Error Messages" section in Appendix A contains expanded explanations of the errors encountered.

12 Concluding Remarks

The development of COMMIX began in 1976, with emphasis on the analysis of fuel assemblies, specifically under natural-circulation conditions. However, as the development progressed and the structure of COMMIX started to evolve, it became apparent that COMMIX could be made a user-oriented general-purpose code with a wide range of capabilities and applicabilities.

The new development of COMMIX then became a continuously evolving dynamic process. New modifications and improvements were implemented continuously in response to

- New physical models, and solution procedures.
- · Feedback from users, and
- A desire to streamline the code, make it more use. priented, and increase its generalities and capabilities.

The first version of COMMIX, named COMMIX-1, was released in March 1978. Development then continued and many more features were added, e.g., thermal- and force-structure models, a cylindrical geometry option, semi-implicit and fully implicit solution procedures, etc. In December 1983, COMMIX-1A was released. Further development led to COMMIX-1B, which was released in September 1985 and included new features such as turbulence models and a volume-weighted skew-upwind difference scheme. Since then, we have added many more features and refinements and we release it now as an extended version called COMMIX-1C.

Since the inception of COMMIX development, code verification has been performed in parallel with development. Extensive simulations have been performed to check and verify every step of development. It is generally felt that COMMIX is a very well tested computer code. However, because COMMIX is so large and general-purpose, some bugs might have been overlooked. We certainly welcome feedback from any user who may encounter a bug or who has suggestions on improving the COMMIX code.

Within the constraints of available time and manpower, we have made very effort to make COMMIX a well-tested, user-oriented computer code. But there still are many more improvements that could be implemented to make it even more user-oriented. The following are examples:

- Implement more error detections and diagnostics to provide information that will guide the user through abnormal terminations.
- Develop a software package for computing all geometry-related information (e.g., mesh size, volume and directional surface porosity, and surface area) and generating input for COMMIX.
- Develop an interactive input processor for auxiliary input information, e.g., boundary conditions, thermal structures, and force structures.
- Develop a postprocessor for connecting COMMIX output to plot processors for generating vector and isotherm plots.

If time and program funds permit, efforts will be made in these directions.

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Appendix A: Input Description

A.1 General Comments

Throughout this document, all words corresponding to FORTRAN statements or keywords appear in the Courier Bold font. Default values are indicated by an asterisk or a value in parentheses after the variable description. Arrays are indicated by a subscript following the variable name.

A.2 Some Terminology

The computational domain is partitioned into a number of computational cells, each bounded by consecutive \mathbf{x} -, \mathbf{y} -, and \mathbf{z} -direction (or \mathbf{r} -, $\mathbf{\theta}$ -, and \mathbf{z} -direction) grid planes. Surfaces (portions of a plane or cylinder) may be defined both on the exterior, bounding the computational domain, and in the interior. The intersection of a surface and consecutive grid planes outlines a surface element. Surfaces that coincide with a grid plane are called regular surfaces; otherwise, they are called irregular surfaces. A regular cell is one with all faces coinciding with grid planes. Irregular cells have one irregular surface element.

A.3 General Input Structure

User input is read from a file associated with unit 5. This input consists of two required namelists, optional namelists, and several other record groups. The term record refers to a string of ASCII characters terminated by a carriage return or \n. This corresponds to the earlier concept of a card image. The user may specify unit 5 input in any order. One possible order follows:

Problem Description and Comments	(Optional)
Namelist/geom/	
Namelist/data/	
Boundary Surface Identification Records	(istate = 0)
Cell Initialization Records	(Optional)
Surface Element Initialization Records	(Optional)
Force Structure Specification Records	(Optional)
Thermal Structure Location Records	(Optional)

A.4 Input

A.4.1 Problem Description and Comments

To sense the presence of optional input, columns 1-4 of each line of input are compared with the key words listed below. When a match is found, the line is reread in the appropriate format. If no match is found, the line is ignored or, in effect, treated as a comment. Thus, any number of user comments can precede namelists or be interspersed between non-namelist input as long as columns 1-4 do not contain any of the keywords.

al	alx	aly	alz
ireg	reg	in	out

flow	pold	qbn	qsou	
hl	hlb	rlb	tl	tlb
td	tdb	tk	tkb	
ul	v1	w1	velb	
xfor	yfor	zfor		
6 t	& f	& m		

A.4.2 Namelist/geom/

The variables listed below are used to determine the amount of memory to be allocated for the run. It is important that they be specified correctly. The variables preceded by an asterisk can be approximated by a value larger than actually needed. The minimum values are printed after they are computed. Any of these variables that remain unchanged for a subsequent restart run need not be respecified because they are read from the restart file.

*nm1	*n11	nsurf	
1 max	jmax	kmax	
nforce	iturke	istruc	igeom
nnzero	nnon0	nspace	ilmax

The first three variables listed below can be set to allow for more efficient computation when running one- or two-dimensional problems.

ifx	1	Perform all x-component calculations. (*)
	0	Bypass x-component calculations.	

- 1 Perform all y-component calculations. (*)
 O Bypass y-component calculations.
- 1 Perform all z-component calculations. (*)
 O Bypass z-component calculations.
- 1 Geom O Regular Box geometry (Cartesian coordinate) option. (*)

 -1 Cylindrical geometry option using box geometry input.

 Note 1: A surface must be dedicated to $\mathbf{r} = 0.0$ when the origin is present. Set kflow(n) = -3 and ktemp(n) = 400 for that surface.

 Note 2: For full 2π radian geometries, $\mathbf{j} = 1$ and $\mathbf{j} = \mathbf{jmax}$ are automatically linked; thus, no surfaces need be defined at θ (y) = 0.0 and θ (y) = 2π .

Flag to determine the solution technique used to solve the transport equations. These include energy, turbulent kinetic energy, and turbulent dissipation. (0)

O Successive overrelaxation (SOR) solution scheme is used. Values for eps1 and omega must also be specified when using this option.

The Yale Sparse Matrix Package (YSMP) solver is used. This option is recommended when the number of computational cells, nml, is less than 1000. Values for nnzero and nspace are required when using this option.

(*)

Flag to determine the solution technique used to solve the pressure equation.

O Successive overrelaxation (SOR) solution scheme is used. Values for eps1 and omega must also be specified when using this option.

- 1 The Yale Sparse Matrix Package (YSMP) solver is used. This option is recommended when the number of computational cells, nm1, is less than 1000. Values for nnzero and nspace are required when using this option.

 (*)
- The preconditioned conjugate gradient solver is used. This option is recommended when the number of computational cells, nm1, is greater than 1000.

n11 Total number of surface elements. (0)

Note. Both nl1 and nm1 can be approximated by values larger than actually required. However, if this is done, they must not be included in namelist/geom/ when restarting (istate > 0). Storage will be allocated according to the values specified in the input rather than the minimum storage needed. The minimum values are printed when computed. If one desires to change nl1 and/or nm1, it must be done only at the start of a steady-state run (istate = 0).

The required values for the following variables are internally computed during initialization for a problem. If the input values are too small, the run will terminate with a message indicating the proper size for these variables.

nnon0 Number of matrix non-zeros.

nnzero Number of matrix non-zeros when using YSMP.

nspace Work space size when using YSMP.

ilmax Maximum number of surface elements on any surface.
(2*max(imax, jmax, kmax))

A.4.2.1 Restart Option

When ifres is set to either 1 or 3, there are two ways to force the code to write a restart file. The first is to specify the amount of CPU time in seconds allowed for the run in the variable trest. The amount of CPU time used is checked at the end of each iteration using the Sun FORTRAN library routine dtime. If the number of CPU seconds is less than trest, another iteration is performed. If not, a restart file is written. Both ntmax and timax must be set to large values when using this option. The second way to obtain a restart file is to set ntmax or timax to a simulation time step or simulation time that will be reached before the trest seconds of CPU time have been used. A restart file will be written at this time step or time. After a restart file is written, execution terminates. When restarting from a previous run, make sure that istate is set to the appropriate value. Also, it is advisable to delete all input for variables that one does not intend to change. In some cases, variables will be reset to their initial values if the input specification remains in the input stream. In short, the minimum input necessary is the correct input for restart cases.

ifres O New case with no restart written. (*)

1 New case with restart written to unit 10.

2 Restart of previous run read from unit 9 with no restart written.

3 Restart of previous run read from unit 9 with restart written to unit 10.

In COMMIX-1C, two turbulence models are included. For all of the details of iturke input requirements for these options, see the Turbulence Models in namelist/data/. Constant Turbulent Viscosity Model. (*) 0 12 K-E Turbulence Model. Number of force structures. (0) When nforce > 0, both the Forcenforce Structures section of namelist/deta/ and the Force-Structure Specification Records are required. No thermal structures are used. (*) Do not include inermal-Structure input istruc or Thermal-Structure Location Records in the input. Thermal structures are used. Namelist/struct/. Thermal-Structure input, and Thermal-Structure Location Records are required in the input. The storage layout table is not printed. (*) istbug The storage layout table is printed. The input file listing is suppressed. -1 The Boundary Surface Summary is not printed. (*) 0 ibsbug The Boundary Surface Summary is printed, after which execution continues. For a description of the Boundary Surface Summary, see Sec. A.10 "Finding Holes in the Boundary" The Boundary Surface Summary is printed, after which execution terminates. The maximum number of cells in the x-direction (x). (1) imax The maximum number of cells in the y-direction (theta). (1) max The maximum number of cells in the z-direction. (1) kmax The number of unique surfaces enclosing the computational domain. Unique nsurf surfaces are determined by a unique combination of the following three characteristics: 1. Velocity Boundary Condition. 2. Temperature Boundary Condition. 3. The unit normal vector to the surface. The computational cell sizes along the x-axis, m. dx(1)The computational cell sizes along the y-axis, m or rad. dy (1) dz(k)The computational cell sizes along the z-axis, m.

The unit normal vectors referred to by the following three variables are those pointing into the computational domain.

morml(n) The x-component of the unit normal vector to surface n.

ynorml (n) The y-component of the unit normal vector to surface n.

znorm1 (n) The z-component of the unit normal vector to surface n.

A.4.3 Namelist/data/

- alpha 0.0 Semi-implicit time advancement for both momentum and energy equations.
 - 1.0 Fully implicit time advancement for both momentum and energy equations. (*)

ifmom O No momentum calculation.

1 Momentum calculation is performed. (*)

ifener O No energy calculation.

1 Energy calculation is performed. (*)

iskew Two numerical schemes are available.

O Pure Upwind Differencing scheme. (*)

- 2 Flow Modulated Skew Upwind Discretization scheme. This option reduces numerical diffusion inaccuracies present in the Pure Upwind Differencing scheme when the predominant flow is not orthogonal to the computational mesh.
- itrans 0 The unsteady term of the momentum equation is evaluated according to Eq. 4.25b of Vol. I.
 - 1 The unsteady term of the momentum equation is evaluated similarly as shown in Eq. 4.23 of Vol. I.

The two variables below give the user some control over the frequency at which the momentum and energy calculations are performed. The need for this control might arise when one of the two fields (relocity or energy) varies slowly compared to the other. The intent is to perform one of the calculations (momentum or energy) at every time step while performing the other only occasionally, resulting in a savings of CPU time. Before the user activates these variables, it is highly recommended that the full implications of this approximation be understood. The following combinations are allowed:

isetmo = 1 and iseten = n

where n is any nonzero integer.

isetmo = n and iseten = 1

where n is any nonzero integer.

isetmo = m and iseten = n

where one of the following conditions is satisfied:

- (1) m < 0 and n divides m or
- (2) n < 0 and m divides n.
- when n is less than zero, the energy calculation is turned off every -nth time-step. When n is greater than zero, the energy calculation is turned on only every nth time-step. (1)
- when n is less than zero, the momentum calculation is turned off every -nth time-step.

 When n is greater than zero, the momentum calculation is turned on only every nth time-step. (1)
- Start of steady-state run. Geometry, boundary conditions, and initial conditions are specified from the input stream. Other parameters take default values or zero. (*)

Continuation of a steady-state run. Initial conditions are read from the restart file of a previous run in which steady-state has not yet been achieved. Some parameters may be changed in the input stream.

Beginning of a transient run. Initial conditions are read from the restart file of a previous run. It is desirable, although not necessary, that this previous run has achieved steady state. Some parameters may be changed in the input stream.

Continuation of a transient run. Initial conditions are read from the restart file of a previous beginning-of-transient run or continuation-of-transient run. Limited changes may be made in the input stream.

No convergence information is printed. 0 itibua Convergence information is printed at every iteration.

The defaults for the following two values are 1 when istate = 0, and 0 when istate = 2. In other cases, these variables are ignored.

No new thermal structure input is read. newts New thermal structure information is read if istruc = 1 and istate = 0 or istate = 2.

No new force structure information is read. newfor New force structure information is read if nforce > 0 and istate = 0 or istate = 2.

A.4.3.1 Time- and Time-Step-Related Parameters

Time-step size for time-steps 1 through lastdt, s. (0.1). This value is used dt (1) only if idtime = 0.

Time-step size for time-steps after lastdt, s. (0.1). This value is used only dt (2) if idtime = 0.

The time-step size is taken from the user-specified variable dt. idtime The time-step size is computed internally as the product of the largest allowable time increment given the conditions (Courant time-step size) and a user-specified variable, rdtime. (*)

No subroutine timing information is shown. (*) itimer Subroutine timing information summary.

Subroutir timing information is shown after every call. 2

This variable in combination with dt allows the user to change the time-step lastdt size during a run. The time-step size for all time-steps through lastdt is taken from dt(1). After step number lastdt, the time-step size is taken from dt(2). (99999) This value is used only if idtime = 0.

Up to 10 values to specify the time-step numbers to call subroutine nthcon gdconv to calculate convergence criteria and the allowable time-step size. The following are acceptable values of nthcon:

O No further calls to gdconv.

No further calls to gdconv.

Time-step number for which gdconv is called. After the nth positive timestep number in ntheon has been processed, the (n + 1)th value of ntheon is used to determine subsequent calls to gdconv.

A value of -n indicates that gdconv is to be called every nth time-step. No subsequent values of nthcon are considered. (-1) See ntprint and ntplot for examples.

The maximum time-step number for this run. Normal termination occurs ntmax after completion of this time step. (99999)

The time-step size is computed internally as the product of the largest edtime allowable time increment given the conditions and the variable, rdtime. (0.8) This value is used only if idtime = 1.

The maximum time of this run. Normal termination occurs after this time timax has been reached, s. (3.6E+7) Timax refers to the simulation or problem time, not the computer CPU time needed to run the problem.

trest COMMIX-1C calls the Sun FORTRAN Library Routine dtime to obtain the

elapsed run time in seconds for the calling process. When, at the end of an iteration, this elapsed time exceeds trest, the calling process is terminated after optionally writing a restart file. (3600.0)

Initial time, s. (0.0) This value should be reset to zero at the beginning of a tstart

transient run, istate = 2.

A.4.3.2 Iteration Control Parameters

The general definitions and default values of control parameters are given in this section. For additional information, see Sec. A.5 "Control Parameters at a Glance" and Sec. A.6 "Steady-State Definition."

eps1	Convergence criterion parameter, (1.0E-4)
eps2	Convergence criterion parameter. (1.0E-6)
ервЗ	Convergence criterion parameter. (5.0E-5)
eps5	Convergence criterion parameter. (1.0E-5)
it(1)	Number of iterations for time-steps 1 through lastit. (10)
it(2)	Number of iterations for time-steps after lastit. (10)
itmaxp	Number of iterations in the pressure iteration loop. (99)
itmaxe	Number of iterations in the energy iteration loop. (99)
lastit	This variable, in combination with it, allows the user to change the number of iterations per time-step during a run. The number of iterations for all time-steps through lastit is taken from it(1). After step number lastit, the number of iterations is taken from it(2). (99999)
omega	Relaxation factor for the SOR pressure solver. (1.5)
omegae	Under-relaxation factor for the energy equation coefficients. (0.8)
omegar	Under-relaxation factor for the density. (1.0)
omega"	Under-relaxation factor for the momentum equation coefficients. (0.8)
relaxe	Relaxation factor for the SOR energy solver. (0.95)

A.4.3.3 Boundary Condition Types

All external surfaces must have a velocity-boundary condition type and a temperature or heat-flux boundary condition type. Internal surfaces may also be assigned boundary condition types.

Type of velocity boundary condition. (The default for all nsurf surfaces is 1) kflow(n)

Continuative mass flow outlet.

Uniform velocity outlet. .4

-3 Free slip boundary.

-2 Continuative velocity outlet.

-1 Continuative momentum outlet.

Solid wall.

- Constant velocity boundary with normal velocity set from veloc(n) or explicitly specified by the Boundary Value Initialization Records. The tangential component is, in effect, zero. (*)
 - Constant mass flow flow = rlb * welbn * area specified by the Boundary Value Initialization Records.
- 100+nf Uniform transient velocity boundary with normal velocity set from the product of the nfth transient function and veloc(n).
- 200+nf Transient mass flow boundary with normal velocity set uniformly from veloc(n)/sum(rlb*area).
- kpres(n) Type of pressure boundary condition. Pressure boundary conditions are
 applied to the cells adjacent and interior to the boundary surface specified.
 (The default for all nsurf surfaces is 0)
 - O No pressure boundary condition is applied. (*)
 - 1 Uniform constant pressure boundary with pressure set from pres(n).
 - 100+nf Uniform transient pressure boundary with pressure set from the product of the nfth transient function and pres (n).
- ktemp(n) Type of temperature or heat-flux boundary condition. (The default for all nsurf surfaces is 1)
 - Specified constant-temperature boundary with temperature set from temp(n) or the Surface Element Initialization Records. (*) The surface heat flux is nominally computed considering the fluid conduction, but not the presence of a wall. To account for both fluid convection and wall conduction, the following variables from the Wall Model section below must be specified: ihtwal(n), walldx(n), and matwal(n).
 - 100+n# Uniform transient-temperature boundary with temperature set from the product of the n#th transient function and temp(n). The surface heat flux is computed with the options as specified above for ktemp(n) = 1.
 - Specified constant-heat-flux boundary with normal heat flux set from temp(n) or the Surface Element Initialization Records.
 - 300+nf Uniform transient-heat-flux boundary with normal heat flux set from the product of the nfth transient function and temp(n).
 - 400 Adiabatic or zero-diffusive heat-flux boundary.

A.4.3.4 Wall Model

When specifying either a constant-temperature boundary condition or a uniform transient-temperature boundary condition (ktemp(n) = 1 or ktemp(n) = 100+nf) a wall may be modeled by defining the following three variables:

- walldx(n) Wall thickness, m. (1.0)
- matwal (n) Material type for surface n. The value of this variable is used as the index nm in the Material Properties section below. (1)
- ihtwal (n) Heat-transfer coefficient number for the calculation of heat-transfer between coolant and wall. The value of this variable is used as the index nh of the variables ihtcor, htclen, and htcmul in the section describing the Fluid-Structure Heat Transfer.

A.4.3.5 Uniform Boundary Initialization

The following three variables allow easy specification of uniform velocity, temperature or heat flux, and pressure values at boundaries. Nonuniform distributions can be specified by _sing the Surface Element Initialization Records.

veloc(n)	Initial velocity at surface n in the direction indicated by *norm1 (n).	
	ynorm1 (n), and znorm1 (n), m/s. (0.0)	

temp(n) Initial temperature for surface n, °C. (0.0) For a constant or transient heat-flux boundary, temp(n) contains the heat flux, W/m². (0.0)

pres(n) Initial pressure for surface n. Pa. (0.0)

A.4.3.6 Uniform Cell Initialization

The following variables allow easy specification of uniform cell temperatures and pressures. Nonuniform distributions can be specified by using the Cell Initialization Records.

temp0	Initial temperature of all internal cells, °C. (0.0)
pres0	Initial pressure at the pressure reference point located at (xpres0,ypres0, zpres0), Pa. (1.01353E+5) The default pressure initialization computes the static head using the density evaluated at temp0, and pres0. The initial static head pressure at any point is computed with respect to the pressure reference point.
xpres0	x-coordinate of the pressure reference point, m. (0.0)
ypres0	Y-coordinate of the pressure reference point, m. (0.0)
zpres0	z-coordinate of the pressure reference point, m. (0.0)
gravx	x-component of gravity vector, m/s2. (0.0)
gravy	Y-component of gravity vector, m/s ² . (0.0)
gravz	z-component of gravity vector, m/s². (0.0)

A.4.3.7 Fluid-Structure Heat Transfer

Fluid-structure heat transfer (g) is computed as follows:

q=A*h*(Ts-Tf)

where

A is the area,

h is the heat transfer coefficient.

Ts is the temperature of the structure, and

Tf is the temperature of the fluid.

Heat transfer coefficient nh. which is specified by the input variables intwal (n) in the Wall Model section and int in the Thermal Structure Fluid Namelist, is defined by three input parameters:

intcor(nh) Heat transfer coefficient correlation number.

htclen(nh) Characteristic length.

htcmul(nh) Heat transfer coefficient multiplier.

When the correlation number, intcor(nh), is in the range of 1 to 10, then the heat transfer coefficient, h, is defined as follows:

h = htcmul(nh)*Nu*k/htclen(nh)

where

ic = ihtcor(nh).

Nu = heatcl(ic)+heatc2(ic)*Re**heatc3(ic)*Pr**heatc4(ic).

Re is the Reynolds number,

Pr is the Prandtl number, and

heatcl (ic) is the Nusselt number coefficient.

Because the Nusselt number, Nu, must always be positive,

heatcl (ic) should be positive to accommodate a zero-flow situation (5.0),

heatc2 (ic) is the Nusselt number coefficient (4.02E-4),

heatc3(ic) is the Nusselt number coefficient (0.8).

heatc4 (ic) is the Nusselt number coefficient (0.0), and

k is the fluid conductivity.

When the correlation number, inter(nh), is in the range of 11 to 20, the heat transfer coefficient, h, is defined as follows:

h = htcmul(nh)*heatcl(ic)+

heatc2(ic)*Re**heatc3(ic)*Pr**heatc4(ic)

where

ic = ihtcor(nh)-10.

A.4.3.8 Material Properties

Material properties are needed when modeling the fluid in the computational cells (matype) and, optionally, walls (matwal (n)). The values of matype and matwal (n) may be any integer from 1 to 24. When the value is in the range of 1 to 20, the material properties are computed from the fast-running simplified approximations to the state equations given below.

Conductivity in W/(m °C)

cond = c0k(ma)+c1k(ma)*tc+c2k(ma)*tc**2

Density in kg/m3

dense = c0ro(ma)+c1ro(ma)*tc+c2ro(ma)*Pa/tk

Enthalpy in J/kg

enth = c0h(ma)+c1h(ma)*tc+c2h(ma)*tc**2+c3h(ma)*Pa

Saturation pressure in Pa

psat = exp(cOp(ma)+tc*clp(ma)+tc*tc*c2p(ma))

Viscosity in Pas

visc = c0mu(ma)+c1mu(ma)*tc+c2mu(ma)/tk

Molecular weight of material ma

molwt = wtmol(ma)

where

to is the temperature in °C.

tk is the temperature in K.

Pa is the pressure in Pa, and

h is the enthalpy in J/kg.

matype

Coded value of material type. The following values of matype are associated with rigorous equation-of-state subroutines. This list may be expanded with little difficulty by users having more accurate equation-of-state subroutines for their materials.

- 21 Water liquid
- 22 Water vapor
- 23 Sodium liquid
- 24 Sodium vapor

tabhit (nm)

mattab (nm) To allow the user to spot-check property values, a small table is printed for tablot (nm) each of the material types listed in the variable mattab, with five temperature values ranging from the corresponding entries in tablot to tabhit at a pressure of preso. Fluid property values are printed when mattab is less than 100. Solid material properties are printed when mattab is set to 100+material type. For example, one could obtain a table of property values computed from the coefficients cOk(1), c1k(1), c2k(1), cOro(1), clro(1), c2ro(1), c0h(1), . . . etc., over a temperature range of 500.0 to 900.0°C and a table of liquid-water property values over the range of 20.0 to 90.0°C by including the following input in namelist/data/:

mattab = 1.21.

tablot = 500.0, 20.0,

tabhit = 900.0,90.0

The default value for each of the above three variables is zero; thus no property tables are printed unless these values are specified.

A.4.3.9 Transient Functions

All transient driving functions are input into the following three variables. They must be input at the beginning of the transient (istate = 2) even if they have been input

previously. Each function is defined by a user-specified set of points. Cubic-spline-fit coefficients are then generated in subroutine fitit. Fifty equally spaced values are printed to allow the user to check the adequacy of the input distribution. Ten to fifteen values with points concentrated at rapidly changing y-values should be adequate. Currently, the total number of points allowed for the specification of transient functions is 100.

tval (np) The independent variable, usually time, for the transient functions.

The dependent variable for the transient functions. The first value of the second function immediately follows the last value of the first function. The same pattern must be followed for all subsequent functions. Make sure that the entire range of the function used lies within the range input because the fitting routine does not extrapolate. Discontinuities are indicated by specifying the same X-coordinate twice with the same or different Y-coordinate values.

nend(nf) The number of points in the nfth transient function.

To simplify thermal structure input in certain cases, the heat-source transient function numbers can be overridden in namelist/data/. These values are input into the variable ntots in the order that the thermal structure prototypes were defined. Any values specified in ntots will override all other input and previous values. If no values of ntots are defined, no changes to the heat-source transient function numbers are made.

Number of the transient function used as a multiplier of the heat source for the coolant when thermal structures are present and as a multiplier of total heat source when no thermal structures are present.

ntplot Up to 25 values to specify when plotting information is to be written to unit 76. The following are acceptable values of ntplot:

O No more plotting information is written to unit 76. (*)

>O Time-step number for which plotting information is written to unit 76. After the nth positive time-step in ntplot has been processed, the n+1th value of ntplot is used to determine which subsequent time-steps are written to the plot file.

A value -n indicates that information is written to unit 76 every nth time step. No subsequent values of ntplot are considered. Example: ntplot = -5 indicates that every fifth step is to be processed. ntplot = 5,10,-20 indicates that steps 5, 10, 20, 40, 60, etc., are to be processed. ntplot = 10,20,0 indicates that only steps 10 and 20 are to be processed.

A.4.3.10 Force Structures

The force structure is a mechanism whereby a drag or resistance force (in Pa/m) can be applied to a fluid flow across a cell face between two computational cells. The location of each force structure, nf, is specified in the Force-Structure Specification Records. The generic force structure applies a resistance of one of the following forms:

drdx = -forcef(nf)*rl*abs(ul)*ul*fcorr/clenth(nf),

dpdy = -forcef(nf)*rl*abs(vl)*vl*fcorr/clenth(nf), or

dpdz = -forcef(nf)*rl*abs(wl)*wl*fcorr/clenth(nf),

where

```
foorr = acorrl(nc) *re*-bcorrl(nc) +ccorrl(nc)
when
    re < reytrn(nc),
and
    fcorr = acorrt (nc) *re**bcorrt (nc) +ccorrt (nc)
when
    re >= reytrn(nc),
given that
    re = rl*sqrt(ul**2+vl**2+wl**2)*reylen(nf)/vis.
where
    rl is the local density.
    ul. vl. and wl are local velocities.
    vis is the local viscosity, and
    no is the correlation index. icorr (nf).
forcef(nf) Force coefficient for force structure nf.
reylen (nf) Length used to compute the Reynolds number for force structure nf, m.
clenth (nf)
       >0.0
               The value input is used as the characteristic length in the above equation.
       < 0.0
               A characteristic length computed from either dx, dy, or dz, whichever is
               appropriate, is used for clenth (nf) in the above equation.
               The correlation index of force structure nf. For the generic force structures, the values of icorr must be less than 21. These values are used
icorr(nf)
               as indices of the user-specified correlation variables below.
               Note: For the valve model, icorr is set to 100 * nv + icorr, where nv is
               the valve number.
               The number of correlation types available for force structures. This value
ncorr
               must equal or exceed the maximum value specified in icorr, but must be
               less than 21.
reytrn (nc) The transition Reynolds number.
acorrl (nc) Correlation coefficients when the Reynolds number above, re, is in the
bcorrl(nc) laminar regime, i.e., when re < reytrn(nc).
ccorrl (nc)
acorrt (nc)
               Correlation coefficients when the Reynolds number above, re, is in the
bcorrt (nc) turbulent regime, i.e., when re >= reytrn (nc).
```

ccorrt (nc)

Pressure Relief Valve

A pressure relief valve can be modeled by specifying a force structure with a correlation index of the form 'vvcc', where 'vv' is the valve number, nv, ranging from 1 to 19, and 'cc' is the correlation index. Associated with each valve, nv, are the following variables:

- ivalve(nv) The state of valve nv. A value of 1 indicates that the valve is open, and a value of 0 indicates that the valve is closed. (0)
- dpopen(nv) The pressure gradient between two cells at which a closed valve opens. Pa.
 (1.0E+20)
- dpclos(nv) The pressure gradient between two cells at which an open valve closes, Pa. (-1.0E+20)

 Note: The pressure gradient between two cells is computed as p(i,j,k)-p(i+1,j,k) for x-direction valves, p(i,j,k)-p(i,j+1,k) for y-direction valves, and p(i,j,k)-p(i,j,k+1) for z-direction valves.

When a valve is closed, a very high resistance is applied across the cell face. When a valve is open, a resistance can be applied in one of two ways:

By specifying a correlation index ic in the range of 1 through 20, one can apply a generic force structure, as defined above. When choosing this option, the user can specify:

```
reylen(nf) = 1.0,
clenth(nf) = alpha, the local volume porosity,
reytrn(ic) = 1.0E+10,
acorrl(ic) = 1/vis, where vis is the local viscosity,
bcorrl(ic) = -1.0, and
```

bcorrl(ic) = -1.0, at ccorrl(ic) = 0.0.

The resistance is then given by

-forcef(nf)*wl.

where w1 is the local velocity.

Alternatively, one can specify a force correlation of 70, and the valve velocity will be computed automatically according to the valve velocity model.

Several other specific structures can be modeled by including a force structure with one of the correlation indices listed in the next section.

Force-Structure Library

Several other specific structures can be modeled by including a force structure with one of the correlation indices listed below.

icorr(nf)
50 dP/dx proportional to velocity (u).

- 60 dP/dx proportional to mass flux (ro*u).
- 61 Specified mass flux, ro*u = forcef(nf).
 90 CRBR fuel assembly.
- 91 CRBR blanket assembly.

92 DRHX (Direct Reactor Heat Exchanger).

93 CRBR chimney assembly.

94 FFTF pin bundles.

95 CRBR control assembly.

96 Axial flow through vertical rod bundles.

- forcef(nf) Force coefficient multiplying the resistance computed for the specific
 structure.
- reylen(nf) When axial flow through vertical rods (correlation index 96) is modeled, this value defines the length used to compute the Reynolds number.

A precise description of the resistance being modeled can be found in the source code for subroutine forces or in the document titled Some Resistance Correlations for COMMIX Users, by Sha and Shah, Argonne National Laboratory Report ATHRP-13 (April 1983).

A.4.3.11 Turbulence Modeling

In all of the following turbulence models, an effective viscosity is uned in the diffusion term of the momentum equation. This effective viscosity is the sum of the turbulent viscosity and the molecular viscosity. Similarly, an effective thermal conductivity is used in the diffusion term of the energy equation, which is likewise the sum of the turbulent thermal conductivity and the molecular thermal conductivity.

Constant Turbulent Diffusivity Model

The turbulent viscosity and turbulent conductivity are assumed constant everywhere.

iturke O Turbulent kinetic energy flag must be zero. (*) Note: The variable iturke must be input in namelist/geom/.

turby Turbulent viscosity, Pass. (0.0) This can be set to some non-negative value.

turbo Turbulent conductivity, W/(m.°C), (0.0)

Two-Equation Turbulence Model

This is the most widely used turbulence model for practical engineering problems. Both the equation for turbulent kinetic energy, tk, and the equation for dissipation of turbulent kinetic energy, td, are solved. Wall-function corrections are applied to cells adjacent to solid walls for both the turbulent kinetic energy equation and momentum equations. Turbulent viscosity is computed with the following equation:

turvis = cdturb*ro*tk**2/td

where

cdturb is the coefficient for computation of shear stress near the wall.

ro is the local density,

tk is the local turbulent kinetic energy, and

td is the dissipation of turbulent kinetic energy.

Note: Values are initialized only when istate = 0 or istate = 2.

For this option, the following input must be specified:

iturke	12	Turbulent kinetic energy flag must be 12. Note: The variable iturke must
be input in namelist/geom/.		be input in namelist/geom/.

akanna	Wall constant.	(0.42)	
akappa	wan constant.	(0.46)	

ct1	Empirical constant used in the equation to compute turbulent kinetic	
	energy. (1.44)	

Temark Maximin monitor of Metations for this patent white of the contract of t	itmaxk	Maximum number of iteration	s for turbulent kin	etic energy equations. '29	11
--	--------	-----------------------------	---------------------	----------------------------	----

omegad	Relaxation factor for equation to compute dissipation of turbulent kinet's
	energy. (0.7)

A.4.3.12 Printed Output

Frequency Control

to subroutine output are controlled by the two variables ntprnt and tprnt. In be used individually or together. The information printed at each call to output rmined by the variables istpr and nthpr, which are described below.

ntprnt

Up to 50 time-step numbers at which subroutine output is to be called. The following are acceptable values for ntprnt:

O No more calls to output. When restarting, previous specification of ntprnt values may be overridden by specifying the desired new values followed by a zero in ntprnt.

Time-step number for which subroutine output is to be called. After the nth positive time-step in ntprnt has been processed, the (n+1)th value of ntprnt is used to determine subsequent calls to output.

A value -n indicates that subroutine output is called every nth time-step. No subsequent values of ntprnt are considered.

-9999

>0

<0

subroutine output is called just before the run is terminated. (*)

Example:

ntprnt = O indicates that after initialization, subroutine output is never
called.

ntprnt = 5.10,-9999 indicates that subroutine output is called at steps
5. 10, and just before termination.

tprnt

Up to 50 times (problem time in seconds) at which subroutine output is to be called. Acceptable values of tprnt follow:

O.O No more calls to subroutine output. (*) When restarting, previous specification of tprint values may be overridden by specifying the desired values followed by a zero in tprint.

>0.0 Times at or after which subroutine output is to be called. When or after the nth positive time in tprnt has been processed, the (n+1)th value of tprnt is used to determine subsequent calls to output.

A value of -T indicates that subroutine output is to be called at T-second intervals. If the nth value is negative, the (n+1)th value stores the next time value at which output is to be called. This is nominally set to zero, but can be specified by the user. No subsequent values of tprnt are considered. Example: tprnt = 1.0,5.0, 10.0 indicates that output is to be called at or after times 1.0, 5.0, 10.0, 20.0, ..., etc. tprnt = -5.0,10.0 indicates that output is to be called at times 10.0,15.0,20.0, ..., etc.

Variable Specification

istpr

Up to 50 coded values that specify the arrays to be printed in the first call to subroutine output. (0)

nthpr

Up to 50 coded values that specify the arrays to be printed in all calls after the first call to subroutine output. For internal arrays, each value of istpr and nthpr is a signed six-digit integer of the form 'svvplll' that is coded according to the rules listed below.

Cell Output

S + Only the plane specified by 'plll' is printed. (*) A plus sign is assumed and need not be specified.

All planes between the values of '111' on the current and following values of istpr or nthpr are printed.

vv 01 ul U-component of velocity, m/s.

02 v1 V-component of velocity, m/s.

03 w1 W-component of velocity, m/s.

04 hl Enthalpy, J/kg. 05 tl Temperature, °C.

06 al Volume porosity.

```
Density, kg/in3.
07 rl
               Static pressure, Pa.
08 p
               Residual mass, kg.
09 dl
               x-direction surface porosity.
10 alx
               Y-direction surface porosity.
11 aly
                z-direction surface porosity.
12 alz
                Density at previous time step, kg/m3.
13 rlold
               Turbulent kinetic energy, J/kg.
14 tk
                Volumetric heat source, W.
15 qsour
                Pressure change from last step, Pa.
16 p-pold
17 p-pstato Pressure minus initial static pressure, Pa.
                Molecular viscosity, Pa·s.
18 rmu
                Pressure minus initial pressure, Pa.
19 p-pres0
                Turbulent conductivity, W/(m.ºC).
20 turcon
                Turbulent viscosity, Pas.
21 turvis
                Molecular conductivity, W/m . C.
22 roon
                U-component of velocity at previous step, m/s.
23 ulold
                V-component of velocity at previous step, m/s.
24 vlold
                W-component of velocity at previous step. m/s.
25 wlold
                Enthalpy at previous step, J/kg.
26 hold
                Static pressure at previous step.Pa.
27 pold
                Fluid cell volume, m3
29 vfluid
                x-direction cell face area, m3.
30 aflux
                Y-direction cell face area, m3
31 afluy
                z-direction cell face area, m3.
32 afluz
                Dissipation of turbulent kinetic energy, W/kg.
37 td
                Coded entries of force structures.
40 iforce
                d(density)/d(pressure), (kg/m3)/Pa.
41 drdp
                d(density)/d(enthalpy), (kg/m3)/(J/kg).
42 drdh
                Mass flow across x-face, kg/s
43 flows
                Mass flow across y-face ,kg/s
44 flowy
45 flowz
                Mass flow across z-face, kg/s
                Kinetic energy, J/kg
46 eke
                Kinetic energy at previous time step, J/kg
47 ekeold
                x-direction mass flux, kg/n2.s.
 48
                Y-direction mass flux, kg/n.2.s.
 49
                z-direction mass flux, kg/m2 s.
 50
```

- p 1 An I-plane is printed.
 - 2 A J-plane is printed.
 - 3 A K plane is printed.
- Specific plane to be _ inted. If s is '+', only one plane is indicated. If s is '-', the '111' values in the current and next values of istpr or nthpr indicate the range of planes to be printed.

Thermal Structure Output

For thermal structure information, each value of istpr and nthpr is a signed six-digit integer of the form 's@nnnn' that is coded according to the following rules:

Only structure number 'nnnn' is printed. (*)
 A plus sign is assumed and need not be specified.

 All structures between the values of 'nnnn' in the current and following values of istpr and nthpr are printed.

nnnn Specific structure to be printed. If s is '+', only one structure is indicated. If
s is '-', the 'nnnn' values in the current and next values of istpr or nthpr
indicate the range of surfaces to be printed.

Surface Element Output

For surface arrays, each value of istpr and nthpr is assigned a six-digit integer of the form 's9vvlll' that is coded according to the following rules:

A plus sign is assumed and need not be specified.
All surfaces between the values of '111' in the current and

All surfaces between the values of '111' in the current and following values of istpr or nthpr are printed.

VV	01	velbn	Normal surface velocity, m/s.
	02	qbn	Normal surface heat flux, W/m2.
	03	mb	Adjacent internal cell number.
	04	hlb	Surface enthalpy, J/kg.
	05	tlb	Surfac temperature, OC.
	06	area	Surface element area, m2,
	07	rlb	Surface density, kg/m³.
	09	ijk	Adjacent internal cell indices. Each value is of the form 'iijjkk', where ii is the i index, jj is the j index, and kk is the k index.
	10	qbn/(tl)	o-t1), W/(m.oC).
	15		Mass flow rate, kg/s.

111 Specific surface to be printed. If s is '+', only one surface is indicated. If s is '-', the '111' values in the current and next values of istpr or nthpr indicate the range of surfaces to be printed.

Example: istpr = 061005,-103001,-103005,

nthpr = 011005,-023001,-023005,901001,-905001,-905005, indicates that the first call to output will print the 1 = 5 plane of volume porosity and k-planes 1 through 5 of the X-direction surface porosity. On all subsequent calls, to output, the I = 5 plane of the u component of velocity, k-planes 1 through 5 of the v component of velocity, the boundary velocity for surface 1, and surface temperature for surfaces 1 through 5 will print.

Output Format Control

ncolum The number of columns to be written in the tabular output. Valid values for ncolum are 8, 9, 10, and 11. The formats used are (1p, 8e13.6). (1p, 9e11.4). (1p, 10E10.3), and (1p, 11e9.2). (10)

A three-digit binary number that determines the row/column orientation of tabular output. The table below gives the acceptable values. (101)

	I-plane	Indices	J-plane	Indices	K-plane	Indices
	Row	Column	Row	Column	Row	Column
000		k	k	1.	1.	3
001		k	k	Δ		1
010	3	k	1	k	1	3
011		k	1.	k	3	1
100	k	3	ĸ	1	1	5
101	k	3	k	1.		1
110	k	3	1	k	ă.	3
111	k	3	1	k	5	1

A.4.4 Boundary Surface Identification Records

These records must be present only at the start of steady-state runs (istate = 0). The purpose of this section is to specify a set of boundary surfaces that completely enclose the computational region and to define any other boundary surfaces inside the computational region. These interior boundary surfaces must completely surround a surface, a cell, or a group of cells. To completely surround a surface, one must specify two boundary surfaces with normals in opposite directions. A single-sided boundary surface is not allowed in the interior of the computational region. Also, be sure that all specified surfaces bound computational cells. Each boundary surface is defined by specifying one or more Boundary Surface Identification Records, each of which contains the following variables in format (a4, f10.3,714):

name area ib ie jb je kb ke n

name	reg	The surface is regular. Regular surfaces lie on grid planes. The surface is irregular. Irregular surfaces do not lie on grid planes.
area	<0.0	Regular Surfaces The area of each surface element of cell (i,j) is set to the product of its actual geometrical value, either $dx(i)*dy(j)$, $dy(j)*dz(k)$, or $dx(i)*dz(k)$, whichever is appropriate, and abs(area). The area of each surface element of cell (i,j) is set to area.
area	<0.0	Irregular Surfaces The absolute value is the slant length. The area of each surface element is set to slant length * delt , where delt corresponds to dx, dy, or dz and is determined by the respective zero-normal vector component. The area of each surface element of cell (i,j.) is set to area.
ib, 16		These six variables are the beginning and ending 1-, 1-, and k-indices that define a rectangular solid composed of one or more cells. The rectangular

kb, ke

solid that defines or partially defines a surface is the one adjacent to and on the side pointed to by the surface normal. (Keep in mind that the surface normals *norml(n), ynorml(n), and znorml(n) to surface n always point into the computational region.) The intersection of each cell and the surface defines a surface element.

n

The surface number. All surfaces with the same combination of the following three characteristics can be assigned the same surface number:

1. Velocity boundary condition.

2. Temperature boundary condition. 3. Unit normal vector to the surface.

Note 1: It is possible for two surface elements to lie in the same surface and have either the same or different surface numbers, as well as for two surface elements to lie in different surfaces and have the same or different surface numbers

Note 2: The order of the Boundary Surface Identification Records must be as follows:

1. All ireg records (irregular surfaces) must precede all reg records (regular surfaces).

2. The surface numbers, n, of all treg records and reg records must be

in the order of increasing value.

Note 3: When cylindrical posturery (igeom = -1) is used, a surface must be specified at the origin when computational cells are bounded by the origin. When an annular region is being modeled, a surface should not be defined at the origin but rather at the boundary of the first (counting from the center) computational cell. Set kflow(n) = -3 and ktemp(n) = 400 for surfaces defined at the origin.

Note 4: When cylindrical geometry (igeom = -1), is used, with 2π radians, j = 1 and j = jmax are automatically linked; thus, no surfaces need be defined

at y = 0.0 and $y = 2\pi$.

A.4.5 Cell Initialization Records

The purpose of this set of records is to permit initialization of internal cell values of any of the arrays listed below. Uniform temperatures can be more easily specified with the variable temp in namelist/data/. Each line in this section contains the following variables according to the format (a4, f10.3, 614):

> nama rval ib ie jb je kb ke

name

Volume porosity, the dimensionless ratio of the fluid volume in a cell to the al total cell volume. (1.0)

hl Enthalpy, J/kg.

pold Pressure, Pa

gsou Volumetric heat source per computational cell volume $dx(1)*dy(j)*dz(k), W/m^3. (0.0)$

Dissipation of turbulent kinetic energy, J/kg. td

tk Turbulent kinetic energy, J/kg,

ti Temperature, OC. (0.0)

rval The value to be assigned to the variable named. These six variables are the beginning and ending i., j., and k-indices that define a rectangular solid composed of one or more cells.

A.4.6 Cell Face Initialization Records

kb, ke

The purpose of this set of records is to permit initialization of internal cell face values of any of the arrays listed below. Each line in this section contains the following variables according to the format (a4, f10.3, 614):

rval ib ie jb je kb ke name name Surface porosity, the dimensionless ratio of the free flow area to the total alx surface element area, between cell (i, j, k) and cell (i+1, j, k). (1.0) Surface porosity, the dimensionless ratio of the free flow area to the total aly surface element area, between cell (1, j, k) and cell (1, j+1, k). (1.0) Surface porosity, the dimensionless ratio of the free flow area to the total alz surface element area, between cell (1, j, k) and cell (1, j, k+1). (1.0) U-component of velocity between cell (1, j, k) and cell (1+1, j, k), m/s. ul (0.0)V-component of velocity between cell (1, j, k) and cell (1, j+1, k), m/s. v1 W-component of velocity between cell (1, j, k) and cell (1, j, k+1), m/s. wl (0.0)The value to be assigned to the variable named. rval These six variables are the beginning and ending i., j., and k-indices that ib, ie define a rectangular solid composed of one or more cells. jb, je Note: When the location of alk(i, j, k), aly(i, j, k), or alz(i, j, k) kb, ke coincides with the location of area(1), the operative variable is area(1). Similarly, when the location of ul(i,j,k), vl(i,j,k), or wl(i,j,k) coincides with the location of velb(1), the operative variable is velb(1).

A.4.7 Surface Element Initialization Records

The purpose of this set of records is to permit initialization of surface element values of any of the arrays listed below. Velocity boundary conditions can be more easily specified using the variable veloc in namelist/data/. Each record in this section contains the following variables according to the format(a4,f10.3,814):

name rval ib ie jb je kb ke n

name

area

Boundary surface porosity, the dimensionless ratio of the free flow area to the total surface element area.

#low

Mass flow through boundary surface element, kg/s.

hlb	Boundary enthalpy, J/kg.
qbn	Boundary heat flux, W/m².
rlb	Boundary density, kg/m ³ .
tdb	Dissipation of boundary turbulent kinetic energy, J/kg.
tkb	Boundary turbulent kinetic energy, J/kg.
tlb	Boundary temperature, °C.
velb	Magnitude of the velocity normal to the surface in the direction indicated by wnorm1 (n), ynorm1 (n), and znorm1 (n), m/s.
rval	The value to be assigned to the variable named.
ib, ie jb, je kb, ke	These six variables are the beginning and ending i j., and k-indices that define a rectangular solid composed of one or more cells. The rectangular solid that defines or partially defines a surface is the one that is totally interior and adjacent to, or partially interior to and intersecting, that surface. Note: The scheme to indicate surfaces in the Surface Element Initialization Records is the same as that used to indicate surfaces in the Boundary Surface Identification Records. Cell surface elements lying on boundaries must be initialized with the Surface Element Initialization Records rather than with the Cell Surface Initialization Records.
n	The surface number of the boundary being set.

A.4.8 Force-Structure Specification Records

These records must be included only when nforce > 0 and newfor = 1 in namelist/geom/.

These records are used to locate the force structures described in the Force Structure section of namelist/geom/. These forces can be applied at cell faces between two computational cells. The locations therefore correspond to portions of grid planes. Each record in this section contains the following variables in the format (a4,714):

name n ib ie jb je kb ke name x-direction force, kg-m/s2. Rfor yfor Y-direction force, kg-m/s2. rfor z-direction force, kg-m/s2. Force structure number. These six variables are the beginning and ending i-, j-, and k-indices used to define a plane of cells. The cell face defined by cell (i,j,k) for an ib, ie jb, je kb, ke x-direction force is that between cells (1, j, k) and (1+1, j, k). For a ydirection force, it is that between cells (1, j, k) and (1, j+1, k), and for a z-direction force, it is that between cells (1, j, k) and (1, j, k+1). The following restrictions apply:

0 < ib <= ie <= imax.
0 < jb <= je <= jmax.
0 < kb <= ke <= kmax, and
0 < n <= nforce.</pre>

A.4.9 Thermal Structures

This section is included if and only if istruc = 1 and newts = 1 in namelist/geom/ and /data/, respectively.

A thermal structure is a collection of thermal-structure elements, each of which has the same characteristics as specified by a thermal-structure prototype. Thermal-structure prototypes are defined using type, fluid, and material namelists with the names t, f, and m, respectively. The order in which these namelists are input indicates the construction of the thermal structures and must conform to the following rules:

- A type namelist must begin the definition of each thermal-structure prototype.
- 2. If fluid interacts with surface one, a fluid namelist must be present after the type namelist (before the first material namelist). If, in addition, fluid interacts with surface two, a fluid namelist must also be present after the last material namelist.
- A gap exists after each material except the last. The gap parameters are specified in the material namelist.
- 4. The initial default for all namelist variables is zero. Subsequent defaults are the values in effect after reading the previous namelist. If, for example, the geometrical type is the same for all thermal structure prototypes, ixyz need be specified only on the first type namelist.
- The definition of thermal-structure prototype n+1 must follow the definition of thermal structure prototype n.
- Null records or records with blanks in columns 1 through 4 may be interspersed as desired.

The precise definition of each namelist is given in the following sections.

A.4.9.1 Type - namelist/t/

- n Thermal-structure prototype number. This number need not correspond to its index or ordinal number.
- ixyz Geometrical type or characteristic.
 - 1 Rods (cylinders) with axis aligned in the 1-direction.
 - 2 Rods (cylinders) with axis aligned in the j-direction.
 - 3 Rods (cylinders) with axis aligned in the k-direction.
 - 11 Slab with normal aligned in the 1-direction.
 - 12 Slab with normal aligned in the 3-direction.
 - 13 Slab with normal aligned in the k-direction.
 - 100 Spheres.
- nt The number of the transient function to be used as a multiplier for the heat source.

rodfr

Rods or cylindrical thermal structures:

- >0 Number or fraction of actual rods interacting with each associated coolant ceil.
- The absolute value is the number or fraction of rods per unit area (m²) normal to the axis interacting with each associated coolant cell. Slab thermal structures:

>0 Slab area in each associated coolant cell, m2.

The absolute value is the slab area divided by the cell area. This value is equivalent to a solid porosity for the structure. Spherical thermal structures:

>0 Number or fraction of spheres interacting with each associated coolant cell.

The absolute value is the number or fraction of spheres per unit volume (m³) interacting with each associated coolant cell.

outr Thermal-structure outer radius, m. Not used for slab-type thermal structures.

A.4.9.2 Fluid - namelist/f/

iht Heat transfer coefficient index. This value is used as the index, nh, in the calculation of the heat transfer coefficient described in the Fluid-Structure Heat Transfer section of namelist/data/.

A.4.9.3 Material - namelist/m/

mi Material type index. This value is used as the index nm described in the Material Properties (Solids) Section of namelist/data/.

Number of partitions in the material. A thermal-structure temperature will be computed for each material partition.

dr Partition size, m.

q Volumetric heat source for the material region, W/m³.

The following gap properties must be correctly specified or defaulted only when another material follows. If a fluid follows, the gap properties are ignored.

sgap Gap size, m. (0.0)

hgap Gap heat transfer coefficient, W/(m2.0C). (1.0)

A.4.9.4 Thermal-Structure Location Records

This section is included if and only if istruc = 1 and wasts = 1 in namelist/geom/.

Once the thermal-structure prototypes have been defined, the location of the thermal-structure elements are specified by the Thermal-Structure Location Records. These records contain the following variables in format (a4,714):

loc num ib ie jb je kb ke

loc out The specified cells interact with the outside or surface 1.

in The specified cells interact with the inside or surface 2.

num Thermal-structure prototype number.

ib, ie jb, je kb, ke These six variables are the beginning and ending 1., 3. and k-indices that define a rectangular (cylindrical) solid composed of one or more cells that are to interact with thermal-structure num.

Note 1: A cell should not be specified twice by the indices unless the true intention is to have two occurrences of the thermal-structure prototype num.

Note 2: Many Thermal-Structure Location Records may be needed to define all the cells interacting with a given thermal-structure prototype.

Note 3: The order in which cells are specified is arbitrary except when the thermal-structure prototype has fluid cells interacting with both surfaces. In this case, cells are paired off in the order in which they are specified. The number of cells interacting with one surface must equal the number of cells interacting with the other surface.

A.5 Control Parameters at a Glance

The table below is included to clarify the role of some of the control parameters. The values indicated, while not guaranteed, are those that have been found to work in many applications. The user is encouraged to optimize these parameters according to application. A single asterisk indicates that the parameter is used. A double asterisk indicates that the parameter is not used. A value enclosed in brackets indicates that the default value is different and that this value must be explicitly specified in the input.

Implicit Time Advancement		Solve	OF	
+Time-step Loop	Default			
ntmax	99999		100	
timax	3.6E+7		-	
lidtime	1		200	
tstart	0.0		100	
1 dt(1)	0.1		**	
dt(2)	0.1		-	
lastdt	99999			
rdtime	[10.0]			
nthcon	-1			
+Outer Iteratio	n Loop			
it(1)	[1]			
1 1 1t(2)	[1]		196	
lastit	99999		-	
1 +Pressure 5	Solver	SOR	YSMP	CCG
omegav	0.8			-
itmaxp	99		**	*
omega	1.5	*	**	**
eps1	1.OE-4		**	
l l eps2	1.0E-6	,	* *	
+Pressure				
+Energy So	olver	SOR	YSMP	
1 I omegae	0.8	-	-	
itmaxe	99	*	**	
relaxe	0.95	*	**	

	eps5 Energy	1.0E-5		**
	omegak itmaxk relaxk eps6	29 0.8	:	YSMP ** **
	omegad itmaxk relaxk eps6 Turbulences	29 0.8 1.0E-5 e Dissipation 5.0E-5 Iteration Loop	SOR * *	YSMP ** **

A.6 Steady-State Definition

Steady-state is reached when the following conditions are met:

- d1 < 1.0, where
 d1 = maximum cell residual/dconv,
 dconv = eps1*(uvwmax+eps2), and
 uvwmax is computed in subroutine gdconv.
- abs(dumax/(velmax*omegav)) < eps3, where dumax is the maximum change of u-velocity component, and velmax is max(vconv. maximum u-velocity component).
- abs(dvmax/(velmax*omegav)) < eps3, where dvmax is the maximum change of v-velocity component, and velmax is max(vconv, maximum v-velocity component).
- 4. abs(dwmax/(velmax*omegav)) < eps3, where dwmax is the maximum change of w-velocity component, and velmax is max(vconv, maximum w-velocity component).
- 5. abs(dh/deltah*omegae) < eps3, where dh is the maximum change in enthalpy over two consecutive steps, and deltah is max(dhconv, maximum current enthalpy variation).

A.7 Error Messages

If something can go wrong, it will, and usually at the worst possible time.

... Murphy

When an error condition is sensed by COMMIX-1C, an error code is printed, along with a brief error message. The following table gives a listing of the error codes and an expanded interpretation of the error condition. In many cases, relevant information is printed out in the line(s) before the error message block.

- ad01 Changes in nm1, nl1, imax, jmax, and kmax are not allowed when restarting (ifres = 2 or ifres = 3).
- ba01 An invalid input parameter has been encountered while initializing cell or surface element values. Numerous conditions can cause such an error; some of them are listed below. One of the following necessary conditions has not been satisfied:

1 <= ib <= imax, 1 <= ie <= imax,

1 <= jb <= jmax, 1 <= je <= jmax,

 $1 \le kb \le kmax$, $1 \le ke \le kmax$,

 $ib \le ie$, $jb \le je$, $kb \le ke$,

0.0 < volume porosity (a1) <= 1.0, or

0.0 <= surface porosity (alx, aly, alz) <= 1.0.

The offending line is either printed above the error message box or is indicated with the following string printed at the right of the line:

'<--**ERROR**

In both cases, the input line is ignored.

- ba02 The surface indicated on a Surface Element Initialization Record has no surface element or area
- bo01 One of the indices of the above Boundary Surface Identification Record is outside one of the following ranges:

1 <= i <= imax, 1 <= j <= jmax1 <= k <= kmax, 1 <= n <= nsurf

or one or more of the beginning indices is greater than the corresponding ending index, i.e.,

ib > ie, jb > je, or kb > ke.

- bo02 On Boundary Surface Identification Records, surfaces must be specified so that surface numbers are in increasing sequential order.
- bo03 Surface specification input error.
- bo04 On Boundary Surface Identification Records, surfaces must be specified, with all irregular surfaces preceding regular surfaces.
- bo05 While processing the record printed above the error box, a surface element was found to be specified as contained in two surfaces.
- bo06 Surface specification input error.

- bo07 The number of surface elements has exceeded the value of nl1 as specified in namelist/data/. If the input value is correct, check the Boundary Surface Identification Records for possible errors.
- boos The number of cells has exceeded the value of nm1 as specified in namelist/data/. If the input value is correct, check the Boundary Surface Identification Records for possible errors.
- cg01 Conjugate gradient option will not work for a cylinder with less than three angular divisions if cylindrical wraparound exists.
- dc01 idtime = 0 or 1.
- dc02 ifmom = 0 or 1.
- dc03 ifener = 0 or 1.
- dcO5 Incorrect values have been specified for iseten and/orisetmo. See namelist/data/ for a description.
- dc06 0 <= istate <= 3.
- $dc06 0 \le istate \le 3.$
- dc07 iskew = 0 or 2.
- erO1 Only 15 calls to errors are allowed before termination. This number can be increased by changing the value of nealls in subroutine errors.
- fm01 The Boundary Surface Identification Records have defined a single-sided interior
- fm02 boundary surface between the indicated cells. Check that all surfaces you have
- fm03 defined bound computational cells. Also be sure that any interior surface has
- fm04 computational cells on both sides. Reread the Boundary Surface Identification
- fm05 Records input section and check your input. Execution continues, but, subsequent
- fm06 results are questionable.
- fm07 Time has run out while attempting to number the cells in fillm. This probably has been caused by an input e ror in the Boundary Surface Identification Records. The maximum time allowed (currently 1000 seconds) can be changed in fillm.
- fm08 One of the following indices is outside of the expected range:

1 <= i <= imax, 1 <= j <= jmax 1 <= k <= kmax

This error usually occurs when the Boundary Surface Identification Records have left a hole in the boundary. Recheck the Boundary Surface Identification Records for an undefined or incorrectly defined surface, and see Sec. A.9 ("Finding Holes in the Boundary").

- fm09 The total number of cells counted in fillm has exceeded the upper bound of imax*jmax*kmax. Recheck the Boundary Surface Identification Records.
- fm10 Excessive wraparound in the theta direction. Recheck the Boundary Surface Identification Records. Also ensure that all surface normals are pointing into the computational domain.
- fm11 The number of cells has exceeded the value of nm1 as specified in namelist/data/. If the input value is correct, check the Boundary Surface Identification Records for possible errors.
- foO1 Invalid initial valve position has been reset to closed (0).

- fo02 An invalid valve position was specified in the variable ivalve. Execution continued after setting ivalve = 0 and force = -1.0E+20.
- fo03 A negative velocity was returned from the subroutine to determine the velocity through a valve. Execution terminates.
- fo04 An invalid correlation was specified for a force structure. Execution continues after setting *force = -1.0E+20.
- gcO1 igeom = 0 or -1.
- gc02 0 <= ifres <= 3.
- gc04 0 <= itimer <= 2.
- gc05 0 <= 1max <= 99.
- gc06 0 <= jmax <= 99.
- gc07 0 <= kmax <= 99.
- gc08 0 < nsurf.
- gc09 istruc = 0 or 1.
- ginO1 dx(1), dy(j), and dz(k) must be nonzero for i = 1 through imax, j = 1 through jmax, and k = 1 through kmax.
- gm02 The length of the normal vectors defined by xnorml(n), ynorml(n), and znorml(n) must be within 1% of 1.0 for irregular surfaces.
- gm03 The length of the normal vectors defined by xnorml(n), ynorml(n), and znorml(n) must be within 1% of 1.0 for regular surfaces.
- ht01 A heat transfer coefficient index of zero has been found. Review the values of int in namelist/f/ of the Thermal-Structure input.
- ifOl An invalid input record has been encountered in subroutine inforc while reading the Force-Structure Specification Records. The first field must contain either 'xfor', 'yfor', or 'zfor'. The following restrictions also apply:
 - 0 < ib <= ie <= imax.
 - 0 < jb <= je <= jmax,
 - 0 < kb <= ke <= kmax, and
 - 0 < nf <= nforce.

The invalid record printed above the message is ignored, and execution continues.

- ifO2 A previously defined force-structure location has been overwritten. In the preceding lines, the first field shows the cell face on which the force structure was being defined, and the second field is the force-structure number, followed by the cell indices. The last force structure defined at a cell face will be the one that is used.
- inO1 Incorrect values have been specified for iseten and/or isetmo. See namelist/data/ for a description.
- Istate has been found to be 0 while attempting to restart from a previous run. It has been reset by the code to 1. Verify that this is an acceptable fix. Execution continues.
- in 03 New thermal structure input will be read. All previous thermal-structure information from previous runs will be ignored.

- inO4 New force-structure information will be read. All previous force-structure information from previous runs will be ignored.
- inO5 W11 and nm1 must not be specified in namelist/geom/ when restarting from a previous run with istate > O. They have been reset to the old values. Verify that this is acceptable.
- inO6 The transient duct wall temperature boundary condition is not available in this version. Use ktemp(ns)=400 and Thermal Structures to model equivalent thermal effects.
- isO1 The Thermal-Structure Location Record printed above the error message box
- isO2 includes a cell within the ranges of the indices but that is not a valid computational cell. The indices of the invalid cell are printed after the Thermal-Structure Location Record. This cell is ignored and execution continues. The results that follow are likely to be incorrect.
- When computing areas and volumes of the partitions of the thermal-structure material regions, an inner radius was found to be less than -1.0E-4*outr, where outr was the outer radius as specified on the Type record. Check the thermal-structure input for outr, dr, and np. If no errors are found here, check the entire input for the thermal-structure prototype. The negative radius is reset to zero, and execution continues. See the following error (1804) for a list of the variables printed above the error block.
- When computing areas and volumes of the partitions of the thermal-structure material regions, an inner radius was found to be larger than the outer radius. Check the thermal-structure input. The inner radius is reset to the outer radius, and execution continues. The parameters printed above the error block are nestructure number, ireg region number, ipar partition number, outr (n) outer radius, dr region size, rout outside radius, and ren inner radius.
- is 05 The heat transfer coefficient number has been incorrectly specified in the Thermal-Structure definition.
- op01 The value printed is an invalid value of istpr or nthpr. The value is ignored, and processing continues.
- op02 A value greater than 50 for vv in either istpr or nthpr has been encountered while printing cell arrays. This value is not currently defined. The value is ignored, and processing continues.
- op03 While attempting to print a surface array, an invalid value of istpr or nthpr was encountered. The value is ignored, and processing continues.
- opO4 A value of O8 for vv in either istpr or nthpr has been encountered while printing surface arrays. This value is not currently defined. The value is ignored, and processing continues.
- op05 A value in the range of 11 to 20 for vv in either istpr or nthpr has been encountered while printing surface arrays. This value is not currently defined. The value is ignored, and processing continues.
- piO1 An invalid value of ncolum has been encountered while printing integer arrays.
 Ncolum must have a value of 8, 9, 10, or 11. Execution continues without printing this table.

- prO1 An invalid value of neolum has been encountered while printing real arrays. Neolum must have a value of 8, 9, 10, or 11. Execution continues without printing this table.
- re01 In attempting to read a restart file, a common block was found to have a length different from that specified on the restart file. This should only occur if changes have been made to the source code of COMMIX. A change of this type will make the changed version of COMMIX incompatible with all previous restart files.
- reO2 In attempting to read a restart file, the portion of common/space/ containing integer arrays was found to have a length different from that specified on the restart file.
- reO3 In attempting to read a restart file, the portion of common/space/ containing real arrays was found to have a length different from that specified on the restart file.
- reO4 While reading a restart file, a difference was found between the force-structure variables expected by the program and those on the restart file. The restart file variables are ignored, and execution continues.
- variables are ignored, and execution continues.

 While reading a restart file, a difference was found between the turbulence model variables expected by the program and those on the restart file. The restart file variables are ignored, and execution continues.
- re06 While reading a restart file, a difference was found between the thermal-structure variables expected by the program and those on the restart file. The restart file variables are ignored, and execution continues.
- re07 in attempting to read a restart file, the portion of common/space/ containing miscellaneous variables was found to have a length different from that specified on the restart file. The restart file variables are ignored, and execution continues.
- slO1 The sodium-property function tliq has failed to converge in 25 iterations. The iteration count, enthalpy, pressure, and last guess of enthalpy are printed. Execution terminates.
- sl02 The sodium-property function soltsa was unable to compute the saturation temperature for the given pressure. The pressure and the last two iterations of saturation temperature are printed. Execution terminates.
- soOl Isolvr must be 0, 1, or 11 through 19.
- 5v01 The sodium-property function sovtem was unable to compute the sodium vapor temperature for the given enthalpy and pressure. The iteration count, enthalpy, pressure, and the last iteration of saturation temperature are printed. Execution terminates.
- ta01 A negative material value mi has been found in the thermal-structure input.
- ta02 When specifying thermal-structure input with igeom = 0 and rodfr > 0, ixyr must be one of the following values: 1, 2, 3, 11, 13, 101, or 103.
- ta03 When specifying thermal-structure input with igeom = 0 and rodfr < 0, ixyz must be one of the following values: 1, 2, 3, 11, 12, 13, 101, 102, or 103.
- ta04 When specifying thermal-structure input with igeom = 0, rodfr must be non-zero.
- ta05 When specifying thermal-structure input with igeom = -1 and rodfr > 0, ixyz must be one of the following values: 1, 2, 3, 11, 13, 101, or 103.
- ta06 When specifying thermal-structure input with igeom = -1 and rodfx < 0, ixyz must be one of the following values: 1, 2, 3, 11, 12, 13, 101, 102, or 103.

- ta07 When specifying thermal-structure input with ageom = -1, rodfr must be non-zero.
- ta08 When specifying thermal-structure input, igeom = 0 or igeom = -1.
- tsO1 When specifying thermal-structure input, type namelists can only appear first, after fluid namelist and after material namelists. Fluid namelists can only appear after type and material namelists.
- ts02 Currently, only 100 thermal-structure prototypes are allowed. If more are needed, changes must be made in common/rebals/ in subroutine alladd and inpstr. Execution terminates.
- ts03 Thermal-structure input processing has been terminated due to errors encountered in the ordering of thermal-structure prototypes. These must be corrected before processing can continue.
- One of the following input rules for the mal structures has been violated: The geometrical characteristics, ixyz, must be one of the following values: 1, 2, 3, 11, 12, 13, 101, 102, 103. Each thermal structure must have at least one material region.
- ts05 An invalid Thermal-Structure Location Record has been found. One of the following restrictions has been violated:

0 < ib <= ie <= imax, 0 < jb <= je <= jmax, 0 < kb <= ke <= kmex, and loc = out or loc = in

or the num value does not match the number of any thermal structure.

- A thermal structure has been encountered with fluid cells interacting at both outside and and inside surfaces, but the number of cells interacting with the outside surface does not equal the number of cells interacting with the inside surface. The four values printed are the structure number, surface interaction code, number of cells interacting with surface 1, and number of cells interacting with surface 2.
- A thermal structure is inconsistent with the Thermal-Structure Location Records. Either the thermal structure specifies only cells interacting with the outside surface and the Thermal-Structure Location Records specify some cells interacting with the inside surface, or the thermal structure specifies only cells interacting with the inside surface and the Thermal-Structure Location Records specify some cells interacting with the outside surface. The four values printed are the structure number, surface interaction code, number of cells interacting with surface 1, and number of cells interacting with surface 2.
- tq01 An invalid value of ixyz has been found in the thermal-structure prototype input with rodf > 0 and rectangular geometry.
- tq02 An invalid value of ixyz has been found in the thermal-structure prototype input with rodf < 0 and rectangular geometry.
- tq03 Rodf has a value of zero in the thermal-structure prototype input for rectangular geometry.
- tq04 An invalid value of ixyz has been found in the thermal-structure prototype input with rodf > 0 and cylindrical geometry.

- tq05 An invalid value of ixyz has been found in the thermal-structure prototype input with rodf < 0 and cylindrical geometry.
- tq06 Rodf has a value of zero in the thermal-structure prototype input for cylindrical geometry.
- tq07 The value of igeom is invalid. Set igeom to 0 or -1 and rerun.
- wl01 The liquid water property function waltsa has encountered a negative pressure when attempting to compute the saturation temperature.
- w102 The liquid water property function walts a has computed a negative saturation temperature.
- zs01 The temperature range for indicated material number has been set to 50.0-90.0 °C. This can be specified by the user in variables tablot and tabhit.
- when using the Simplified Properties Option, you must input nonzero values for comp. clh. coro, and cok. Be aware that the Simplified Properties Option computes properties as a linear function of temperature only, and as such must be used with extreme caution!

A.8 COMMIX-1C Call Graph

The following table indicates the code structure by showing the calling sequence of the subroutines. Calls to function are not indicated. Also, multiple calls may not be indicated.

```
aatitle
| --- runid
    |---idate
    | --- fdate
 ---adrive
    | --- namel
    |---clear
    | ---errors
    | --- alladd
        |---oneadd
         | --- clear
         | --- tscan
            ---errors
            ---namels
    | --- getmem
    | --- stosum
    |---amain
         |---geom3d
            |---namel
            |---boxes
                ---errors
        1
                 | --- ijkset
                |---ijkget
                | --- fillm
```

```
| | | | | | | ---shome
 | | | | | |---ijkget
     | | | |---ijkset
         | |---errors
       | ---errors
       |---inital
       | ---restar
          |---namel
 | |---geochk
       | |---errors
       | |---datchk
   | | | |---errors
          ---errors
          ---sumre2
          --- z s u m
          | |---errors
           |---fitit
          |---inforc
              ---errors
             |---ijkset
           |---inpstr
       | |---namela
             ---errors
          | ---tearea
             | |---errors
             | |---1jkget
          |---ictemp
           |---initpr
           1
             |---ijkget
          ---barin
         | | ---errors
              |---setrm
          | | |---1jkget
         | |---setrl
              | |---ijkget
             |---redef
          ---geovar
         | |---ijkget
           |---initfl
           | |---bcpres
              |---rotemp
              |---getflo
              |---bctemp
              |---bctem0
              |---getrhc
              |---becont
       1 1
              |---bctemt
       1
          1
              | | ---ijkget
```

```
| | |---bcflow
  | |---bcflot
       |---update
       | --- odrv
           | ---mdi
          | ---mdu
          --- SEO
       |---cdrv
          |---nroc
         |---nsfc
          |---nnfc
          |---nnsc
           |---nnto
   |---initur
   | |---turv12
 |---hstruc
 | |---htcoef
| | |---errors
|---tstruc
 | |---ijkget
 | - - - qstruc
 | |---ijkget
|---gdconv
| |---ijkget
   |---setdt
 |---pltape
| |---runid
|---output
| |---global
    | |---runid
   | |---ijkget
   | |---sumrel
     | |---ijkget
   | |---tsq
    | | |---ijkrat
       | |---errors
   ---errors
   |--- outp2
       |---out2
       | |---outiu
       | |---outku
          |---cutju
       | |---chop
     | |---prinro
   | | | ---errors
```

```
| | | | |---outl
  | | | | | |---outfie
              | ---chop
                |---prince
             |---ijkget
          | | |---outfil
             | |---chop
              | |---prinri
             | | |---errors
             |---errors
         |---rsurfo
          |---isurfo
      | | |---ijkget
      | |---pstruc
       |---watstp
      |---setdt
      |---timstp
      | |---update
       | |---bcpres
       | |---bctem0
      | |---htcoef
       | | |---ijkget
          |---getrhc
          |---moloop
          | |---bcflot
          | |---getvis
          | |---xmomi
          | | |---ijkget
              | |--- zmom z
              | --- z m o m x
              | | |---wlfncv
              | |---forces
              | |---errors
              | | |---vstar0
              |---ymomi
              | |---ijkget
              | --- z m o m z
              | | --- z m o m x
              | |---forces
              |---zmomi
             | |---ijkget
                 | - - - z m o m z
                ---zmomx
              | |---forces
              |---peqn
          | | |---ijkget
          | |---solver
   | | | | |---solvit
```

```
| | | | | |---ysmp
| | | | | | |---cdrv
       | | |---ograd
              | |---gnzero
                |---getka
                |---loada
       | | | |---cgsolv
       | | | | |---ilufac
             | | |---ginv
             ---errors
       | |---momeni
          |---getflo
          | --- boflow
    | |---beturb
  | |---tkloop
    | | |---tksorc
       | | |---ijkget
    | | | |---velcen
             |---tkgrad
          | | |---velcen
          |---encon0
         | |---ijkget
         |---tkener
          | |---ijkget
         | |---diffx1
       | |---solver
       |---tdloop
       | |---encon0
         |---tdener
       | | |---ijkget
    | | | |---diffx1
          |---solver
     |---turv12
       |---enloop
    | | |---geteke
         | |---ijkget
         |---bctemt
          |---hstruc
         |---esorce
          | |---qstruc
         | |---ijkget
          1 --- getcon
         |---encon0
         |---encon2
          | ---encx2
         | |---encfy
       | | | |---encor3
   | | | |---ijkget
   | | |---extors
```

1	1 1	energi
1	1 1	ijkget
1	1 1	econdx
1	1 1	gethl
1	1 1	solver
1	1 1 -	rotemp
1	1 1	propf
		getvel
1		bccont
1	1 1	botemp
1	1 1	boflow
1	1 1	tstruc
1	1 1	restar
1	1.1	pltape
1	1 1	errors

A.9 Use of Non-ANSI Extensions to F77

COMMIX-1C is written in FORTRAN 77, with the following non-ANSI extensions:

- 1. Lower-case letters are used to avoid the agony of dealing with upper case text when using the Unix editor vi. The only impact of this convention is the need for the input files to be in the same case as the FORTRAN source because some comparisons are made between strings in the input file and strings defined in the source. If conversion to upper case is desired, be sure that the input data files are also written in upper case.
- 2. The namelist extension, available on most compilers, has been used in COMMIX-1C. Commercially available FORTRAN packages can provide the namelist functionality. A locally written package has been used on an earlier version of COMMIX. While not adapted to COMMIX-1C specifically, it could be used as a basis for a COMMIX-1C version. This latter package can be made available if necessary.
- 3. Common blocks are generally stored as separate files and are brought into the source with the use of "include" statements of the form:

include 'space.omn'

- 4. A provision for handling IEEE exceptions is provided on Sun workstations with the inclusion of the ieee_handler function, referenced in subroutine adrive, and the corresponding external functions referenced there. This provision may be removed or replaced with the appropriate exception-handling facilities of your machine.
- Pointers are used in several subroutines to simplify the dynamic allocation of memory.
 The same effect could be achieved by using the intrinsic location function 10c.
- The intrinsic function loc, which returns the address of the argument, is a
 nonstandard intrinsic that may have a different name and different characteristics on
 other systems.

- 7. The intrinsic function malloc is used in subroutine getmem to simplify the dynamic allocation of memory. On the Sun system, this function allocates an area of memory and returns the address of the start of that area. The argument of the function is an integer specifying the amount of memory to be allocated, in bytes. If successful, it returns a pointer to the first element of the region, otherwise it returns an integer 0. The same effect could be achieved with the use of the location function loc.
- 8. All timings in COMMiX-1C are obtained from subroutine deltat which calls the function dtime from the Sun FORTRAN library. Dtime returns the elapsed time since the last call to dtime or the start of execution on the first call. The argument array returns user time in the first element and system time in the second element. Elapsed time, the returned value, is the sum of user and system time. Deltat returns the elapsed time since the last call as the function value and the cumulative time in the argument runt.

A.10 Porting COMMix-1C to the Cray

Porting the Sun version of COMMIX-1C to the Cray XMP-14 with the CFT77 compiler here at Argonne was a relatively simple task. On the initial port, no efforts were made to vectorize the program. The following issues were addressed:

- Because the word length on the Cray is 60 bits, compared to 32 bits on the Sun, the entire program can be run in Cray single precision. The following changes are required:
 - 1.1 Remove or comment out the contents of the file double.cmn.
 - 1.2 Remove the double precision declaration from all functions.
 - 1.3 The variable 1 must be changed from double precision to real in subroutines cgrad, conres, and minres.
 - 1.4 The ysmp package must be changed from double precision to real (single precision). Instructions to carry out this task are included in the ysmp file.
 - 1.5 Set nobpi, nowpd, and nowps to 1.0 in subroutine adrive.
- The Cray heap allocation library routine, hpalloc, is recommended to replace the Sun memory allocation function malloc.
 - Conversion from malloc to hpalloc were required in subroutines cgrad, conres, jacobi, and minres.
 - 2.2 Modifications to subroutine getmem.
- 3. References to the ieee handler in subroutine adrive were removed.
- The timing function deltat was changed to use the Cray function second rather than the Sun function dtime.

A.11 Finding Holes in the Boundary

The Boundary Surface Summary is intended to help the user find holes in the boundary surfaces. It is obtained by setting ibsbug in namelist/geom/. The boundary surface summary consists of two parts. First is a table of binary strir gs and their corresponding printed characters. Following this table are jmax planes, w''n each computational cell represented by one of the characters from the first table. The binary string associated with each character indicates the location of the surface elements, as described below.

Each bit in the binary string corresponds to a face of the computational cell. The first bit corresponds to the face in the 1- direction; this is the surface between cell (i,j,k) and cell (i-1,j,k). The second bit corresponds to the face in the 1+ direction, the third in the j-, the fourth in the j+, the fifth in the k-, and the sixth in the k+ direction. A surface element is defined at a cell face if the bit corresponding to that face has a value of 1. For example: suppose "F" is printed at the location for cell (i,j,k). "F" corresponds to the binary string "011000." This indicates that a surface element has been defined in the i+ and j- directions, that is, between cells (i,j,k) and (i+1,j,k) and between cells (i,j,k) and (i,j-1,k).

For this scheme to be effective, the table should contain 62 different printable characters. A blank corresponds to string "000000," and string "111111" should never occur. While a laser printer with both upper and lower case is available at Argonne, the printers usually used are impact printers with only about 58 different characters. Therefore, the current implementation uses the character "?" to correspond to all of the following binary strings: "111110," "111101," "111011," "110111," "101111," "011111," and "111111." This does introduce some ambiguity, but the impact is probably not serious. For those users who wish to eliminate these duplications, changes must be made in subroutine shome.

Appendix B: List of COMMIX-1C Subroutines

Subroutine	Calling Subroutine	Descriptions
AATITLE		Writes the title and calls ADRIVE.
ADRIVE	AA'ı.	Opens the necessary files and calls the main program AMAIN.
ALLADD	ADRIVE	Computes addresses of variables according to the key variables read from input.
AMAIN	ADRIVE	Main calling program. See overall flow chart, Fig. 1.
BARIN	INITAL	Reads the boundary and internal cell initialization cards.
BCCONT	INITFL TIMSTP	Updates boundary values on continuative exits.
BCFLOT	INITFL MOLOOP	Updates boundary velocities on surfaces with transient flow boundary condition.
BCFLOW	INITFL TIMSTP MOLOOP	Updates boundary velocities during iterations.
BCPRES	INITFL TIMSTP	Sets specified pressure values at cells adjacent to surface having pressure boundary conditions.
ВСТЕМР	INITFL TIMSTP	Updates boundary values of heat flux, temperature, density, and enthalpy.
ВСТЕМТ	INITFL ENLOOP	Updates boundary values of temperature, pressure, and density for constant and transient heat flux boundary conditions.
ВСТЕМ∅	INITFL TIMSTP	Computes boundary values of pressure, heat flux, and density for constant or transient temperature boundary conditions.
BCTURB	TIMSTP	Updates boundary values of turbulent kinetic energy.
BOXES	GEOM3D	Reads surface specification cards input for the box geometry option.
CGRAD	SOLVER	Solves matrix equation using preconditioned conjugate gradient method.

Subroutine	Calling Subroutine	Descriptions
СНОР	OUT2 OUT1 OUT11	Resets the beginning and end row and column markers to print out only rows and columns containing cell or boundary values.
CLEAR	ADRIVE ALLADD	Zeros out the values of all variables between the two arguments passed.
DATCHK	INITAL	Checks validity of input in NAMELIST/DATA/.
DIFFX1	TDENER TKENER	Computes diffusion between two adjacent cells.
ECONDX	ENERGI	Computes conduction between two adjacent cells.
ENCFY	ENCX2	Computes y-direction weighting factors for flow-modulated skew-upwind difference scheme.
ENCONØ	TKLOOP TDLOOP ENLOOP	Compute upwind convective terms.
ENCON2	ENLOOP	Computes convective flux for flow-modulated skew- wind difference scheme.
ENCOR3	ENCX2	Computes corner weighting factors for flow-modulated skew-upwind difference scheme.
ENCX2	ENCON2	Computes coefficients due to positive x direction for flow-modulated skew-upwind difference scheme.
ENERGI	ENLOOP	Computes coefficients of the energy equation.
ENLOOP	TIMSTP	Calls required subroutines in sequence for solution of energy equation.
ERRORS	Several	Processes error conditions and prints error messages.
ESORCE	ENLOOP	Computes the source term for energy equation.
FILLM	BOXES	Initializes the cell and adjacent cell pointers.
FITIT	INITAL	Computes the coefficients of cubic spline fit for input transient functions.
FORCES	XMOMI YMOMI ZMOMI	Computes user-imposed drag forces.
GDCONV	AMAIN	Computes DCONV, the convergence criteria based on maximum velocity in the region.

Subroutine	Calling Subroutine	Descriptions
GEOCHK	INITAL	Checks validity of input in NAMELIST/GEOM/.
GEOM3D	AMAIN	Determines essential geometric information.
GEOVAR	INITAL	Computes cell volumes and surface areas that remain constant throughout a calculation.
GETCON	ENLOOP	Computes effective thermal conductivity.
GETEKE	ENLOOP	Computes flow kinetic energy.
GETF	several	Determines value of transient function NF at current time
GETFLO	SOLVER INITFL	Computes mass flow.
GETHL	ENLOOP	Computes enthalpy.
GETMEM	ADRIVE	Allocates memory dynamically.
GETRHC	INITFL TIMSTP	Computes boundary density and enthalpy.
GETVEL	TIMSTP	Adjusts velocity after density change.
GETVIS	MOLOOP	Computes effective viscosity for all cells.
GLOBAL	OUTPUT	Prints giobal balances.
HSTRUC	AMAIN ENLOOOP	Computes heat transfer coefficients for thermal structure elements.
HTCOEF	HSTRUC BCTEMØ	Computes heat transfer coefficient.
ICTEMP	INITAL	Initializes default boundary temperature and boundary velocity (or mass flow).
INFORC	INITAL	Reads input related to force structure and prints corresponding input summary.
INITAL	AMAIN	Calls required subroutines in sequence to initialize internal-cell and boundary values of all variables.
INITFL	INITAL	Initializes all fluid variables.
INITPR	INITAL	Sets default static pressure.
INITUR	INITAL	Performs turbulence model initialization.

Subroutine	Calling Subroutine	Descriptions	
INPSTR	INITAL	Reads thermal structure input data, computes required geometrical and physical information, and prints therma structure input summary.	
ISURFO	OUTPUT	Prints surface array IVAR for surface number NSUR.	
MOLOOP	TIMSTP	Calls required subroutines in sequence to solve mass- momentum equations.	
MOMENI	MOLOOP	Calculates new-time velocity using new-time values of pressure.	
NAMEL	GEO3D INITAL ADRIVE	Reads namelist information.	
NAMELS	INSPTR TSCAN	Reads namelists T. F. and M for thermal structures.	
ONEADD	ALLADD	Sets the variable name, type, and length as they are allocated.	
OUT1	OUTP2	Writes a plane of values for cell-centered variables.	
OUT11	OUTP2	Writes a plane of integer values for cell-center variables.	
OUT2	OUTP2	Writes a plane of values for face-centered variables.	
OUTFIE	OUT1	Sets up two arrays, VAL and MARK, of sizes NRMAX and NCMAX for cell-centered variables.	
OUTIU OUTJU OUTKU	OUTP2	Similar to OUTFIE for face-centered variables.	
OUTP2	OUTPUT	Prints array information.	
OUTPUT	AMAIN	Prints array information.	
PEQN	MOLOOP	Computes coefficients of pressure equations.	
PLTAPE	AMAIN RESTAR	Writes plotting information.	
PRINRC	OUT1 OUT2	Writes out incoming array.	
PRINRI	OUT11	Writes out incoming integer array.	

Subroutine	Calling Subroutine	Descriptions
PROPF	ROTEMP	Computes properties.
PSTRUC	OUTPUT	Prints temperature fields and heat transfer information relating to thermal structures.
QSTRUC	AMAIN ESORCE	Solves heat conduction equations and computes effective heat source from thermal structures to coolant.
REDEF	BARIN	Redefines porosities and permeabilities that are R dependent for cylindrical geometry.
RESTAR	INITAL AMAIN	Writes or reads a restart dataset.
ROTEMP	TIMSTP INITFL	Determines state of each cell by updating properties.
RSURFO	OUTPUT	Prints specified surface array.
RUNID	ADRIVE GLOBAL PLTAPE	Returns time and version information.
SETDT	AMAIN GDCONV	Set nonzero time-step size (0.001).
SETRL	BARIN	Performs boundary value initialization.
SETRM	BARIN	Performs interior cell value initialization.
SHOME	FILLM	Prints graphical representation of boundary surface identification cards.
SOLVER	MOLOOP TKLOOP TDLOOP ENLOOP	Calls one of three matrix solvers to solve discretized pressure equation and scalar transport equations.
SOLVIT	SOLVER	Solves matrix equation by SOR procedure.
STOSUM	ADRIVE	Computes lengths of variables and prints storage summaries.
SUMRE1	GLOBAL	Reads and stores a set of input.
SUMRE2	AMAIN	Writes control variable summary.

Subroutine	Calling Subroutine	Descriptions
TDENER	TDLOOP	Computes coefficients of ε (dissipation of turbulence kinetic energy) equation.
TDLOOP	TIMSTP	Computes dissipation of turbulent kinetic energy ϵ for two-equation models.
TIMSTP	AMAIN	Calls required subroutines in sequence to bring variable values from time t to time t + Δt .
TKENER	TKLOOP	Calculates coefficients of turbulent kinetic energy equation.
TKGRAD	TKSORC	Computes gradients used in source terms in turbulence equations.
TKLOOP	TIMSTP	Computes turbulent kinetic energy k.
TKSORC	TKLOOP	Computes source terms in turbulent kinetic energy (k) equation.
TSAREA	INPSTR	Computes total heat transfer area between thermal structures and fluids.
TSCAN	ALLADD	Scans thermal structure input to determine amount of storage needed to run the problem.
TSQ	GLOBAL	Computes total heat for each thermal structure.
TSTRUC	AMAIN TIMSTP	Solves heat conduction equation and computes thermal structure temperature, TTS.
TURV12	INITFL TIMSTP	Computes turbulent viscosity and thermal conductivity for $k\text{-}\epsilon$ two-equation turbulence model.
UPDATE	INITFL TIMSTP	Restores previous time-step values to current time-step values.
VELCEN	TKSORC TKGRAD	Computes cell-centered velocity.
VSTARØ	FORCES	Computes local critical velocity for superheated steam.
WLFNCV	ZMOMX	Modifies wall shear stress to account for frictional force.
хмомі	MOLOOP	Computes coefficients of x-momentum equations.
YMOMI	MOLOOP	Computes coefficients of y-momentum equations.

Subroutine	Calling Subroutine	Descriptions
YSMP	SOLVER	Solves matrix equation using Yale Sparse Matrix Package.
ZMOMI	MOLOOP	Computes coefficients of z-momentum equations.
ZMOMX	XMOMI YMOMI ZMOMI	Computes z-x convective and viscous terms of momentum equation.
ZMOMZ	XMOMI YMOMI ZMOMI	Computes z-z convective and viscous terms of momentum equation.
ZSUM	INITAL	Prints property summaries.

Appendix C: Resistance Correlations

C.1 Introduction

This appendix provides a convenient collection of the resistance correlations that are most commonly needed by COMMIX users. It is written with a desire to save the user from having to search the vast literature. It is also hoped that this appendix will serve as a starting reference for new users.

We caution here that the correlations here are not necessarily the only and final relations. We welcome feedback and comments from all users so that we can add other correlations, update the existing relations, and improve the information presented here.

C.2 Axial Flow in Rod Bundle Assembly

C.2.1 Generalized Correlation

· Laminar Flow

For a laminar axial flow in a rod bundle assembly, Rehme and Trippel recommended the following generalized correlation:

$$f = \frac{\Delta p}{L} \frac{d_b}{\frac{1}{2}\rho v^2} = \frac{C}{Re}. \tag{C.1}$$

where C is a geometric parameter, v is the axial velocity, d_h is the hydraulic diameter, and Re is the Reynolds number.

$$Re = \frac{\rho v d_h}{\mu}.$$
 (C.2)

The central, wall, and corner subchannels in a rod bundle assembly are shown in Fig. C.1. The value of geometric parameter C is a function of

- P/D for central subchannel (Fig. C.2).
- W/D for corner subchannel (Fig. C.2), and
- P/D and W/D for wall subchannel (Fig. C.3).

From the values of geometric parameter for various subsections, we can calculate the value of parameter C for the total assembly

$$\frac{1}{C_{tot}} = \sum_{i} \frac{1}{C_{i}} \left(\frac{S_{tot}}{S_{i}}\right)^{2} \left(\frac{A_{i}}{A_{tot}}\right)^{3}, \tag{C.3}$$

where S is the wetted perimeter, A is the flow cross section, subscript i is for the individual subchannel, and subscript "tot" is for the total rod bundle.

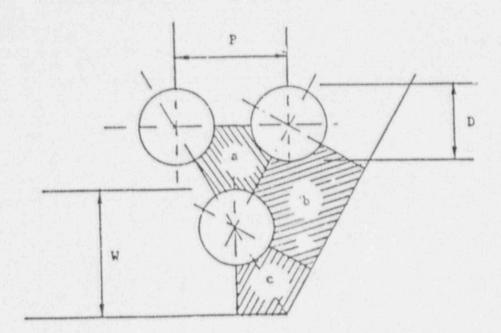


Fig. C.1. Subchannels of rod bundles: (a) central, (b) wall, and (c) corner

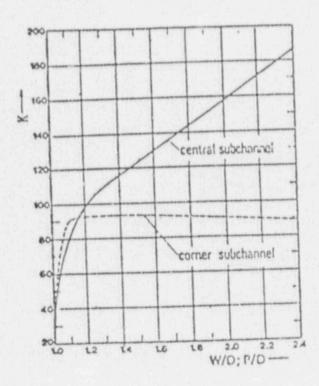


Fig. C.2. Pressure-drop parameter C in central and corner subchannels for lan :ar flow

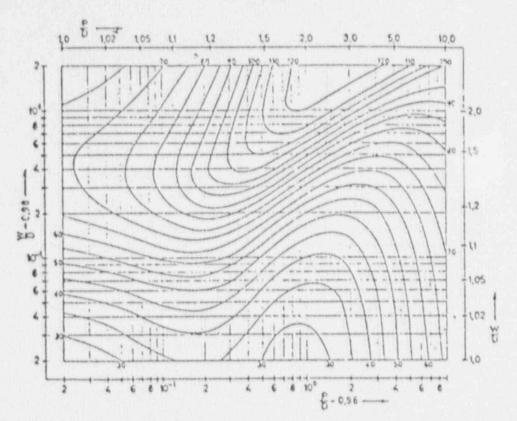


Fig. C.3. Pressure-drop parameter C in wall subchannels for laminar flow

· Turbulent Flow

Rehme² recommended the following equation for the turbulent friction factor in a rod bundle assembly:

$$\left(\frac{8}{f}\right)^{1/2} = A * \left\{2.5 \text{ Log}_{\bullet} \left[\text{Re}\left(\frac{f}{8}\right)^{1/2}\right] + 5.5\right\} - G *.$$
 (C.4)

The two empirical factors, G^* and A^* , are functions of geometric parameter C (Sec. C.2.1), as shown in Figs. C.4 and C.5.

C.2.2 Generalized Correlations for Wire-Wrapped Bundles

Engel, Markley, and Bishop

Based on limited experimental data. Engel, Markley, and Bishop³ recommended the following generalized correlation for a hexagonal fuel assembly applicable in the range $P/D \ge 1.27$ and H < 30 cm:

$$f = \frac{A}{Re} (1 - \chi)^{1/2} + \frac{O.48}{Re^{0.25}} \chi^{1/2} . \tag{C.5}$$

Here.

$$\chi = 0.0$$
 for Re ≤ 400 , (C.6a)

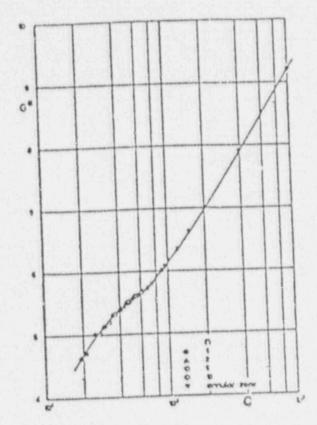


Fig. C.4. Geometric parameter G*

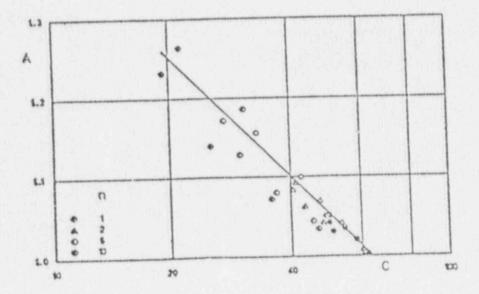


Fig. C.5. Geometric parameter A*

$$\chi = \frac{\text{Re} - 400}{4600}$$
 for 400 < Re < 5000, and (C.6b)

$$\chi = 1.0$$
 for Re ≥ 5000 , (C.6c)

and the coefficient A is a function of wire-wrap lead H and pitch-to-rod diameter ratio.

$$A = \frac{320}{\sqrt{H}} (P/D)^{1.5}. \tag{C.7}$$

Note that the wire-wrap lead H in Eq. C.7 is in centimeters.

· Chan and Todreas

Recently. Chan and Todreas⁴ developed the following generalized correlations applicable to a wide range of wire-wrapped hexagonal fuel assemblies:

$$f = \frac{C_{10}}{Re}$$
 (for Re ≤ 400), and (C.8)

$$f = \frac{C_{12}}{Re} (1 + C_{18} Re^{1.222})^{0.671}$$
 (for Re > 400). (C.9)

Here, Re (=pud_h/ μ) is the bundle Reynolds number and the coefficients C_{18} and C_{19} are functions of the number of rods in a bundle N, pitch-to-rod (pin)-diameter ratio P/D, and lead-length-to-rod (pin)-diameter ratio H/D.

$$C_{18} = A(N)^{B}(P/D)^{C}(H/D)^{E}$$
 (C.10)

and

$$C_{19} = 251(N)^{0.007} (P/D)^{0.997} (H/D)^{-0.354}$$
 (C.11)

The values of the constants A, B, C, and E are given in Table C.1.

For a hexagonal assembly, the flow area and hydraulic diameter, d_h , can be calculated using the relationships:

Flow Area =
$$\frac{\sqrt{3}}{2} (d_{t-1})^2 - \frac{N\pi}{4} (D^2 + D_w^2)$$
, (C.12)

Perimeter =
$$(2\sqrt{3}d_{f-f})^2 + \pi N(D + D_w)$$
, (C.13)

and

$$d_h = 4 * flow area / perimeter$$
. (C.14)

Here, d_{i-1} is the distance between the flat surfaces of the hexagonal assembly, D is the pin diameter, $D_{\mathbf{w}}$ is the wire-wrap diameter, and N is the number of pins in a bundle.

· Rehme

Rehme⁵ recommended the following correlations for wire-wrapped rod bundles:

Table C.1. Values of constants in Eq. C.10

D ≥ 0.35"	D > 0.35"		
A = 0.00221	A = 0.000584		
B = 0.166	B = 0.185		1. H/D≤4
C = 8.297	C = 8.247	for	2. P/D ≥ 1.2 and H/D ≤ 8
E = -1.4567	E = -1.818		3. P/D ≥ 1.343 and H/D ≤ 12
A = 0.0000395	A = 0.000278		
B = 0.063	B = -0.084	for	others
C = 0.174	C = 0.289		
E = 0.178	E = -0.268		

$$f = F \frac{S_b}{S_t} \left[\frac{64}{\text{Re}\sqrt{F}} + \frac{0.0816}{\left(\text{Re}\sqrt{F}\right)^{0.133}} \right]. \tag{C.15}$$

Here, S_b is the wetted perimeter of a rod bundle (rods and wires). S_t is the total wetted perimeter (rods, wires, and casing), and F is the geometric factor.

$$F = \left(\frac{P}{D}\right)^{0.5} + \left[7.6 \frac{D_{w}}{H} (P/D)^{2}\right]^{2.16}. \tag{C.16}$$

C.2.3 Rod Bundles in Clinch River Breeder Reactor

In the Clinch River Breeder Reactor (CRBR) plant, there are several different types of hexagonal rod bundles. The important geometrical characteristics of these bundles are presented in Table C.2.

· Fuel Assemblies (CRBR, FFTF)

Based on the experimental measurements, 6-9 the following correlations are recommended for CRBR and Fast Flux Test Facility (FFTF) fuel assemblies. The same correlations are applicable to both FFTF and CRBR fuel assemblies, because the geometrical features are the same.

$$f = \frac{84}{R_0}$$
 for $R^- \le 1000$. (C.17)

$$f = f_c \left[1.075 + 0.1876 \left(\frac{1000}{Re} \right)^2 + 0.0801 \left(\frac{1000}{Re} \right)^4 \right]$$
 for Re > 1000. (C.18)

Here, fc is the Colebrook friction factor for a smooth tube.

$$\frac{1}{\sqrt{f_c}} = -0.8686 \, \text{Log}_c \left[\frac{2.51}{(\text{Re}\sqrt{f_c})} \right]. \tag{C.19}$$

Table C.2. Important parameters of CRBR hexagonal assemblies

Assembly	No. of Pins	P/D	H/D	D, mm	D, in	d _h , mm
Fuel	217	1.24	51.74	5.842	0.236	3.254
Blanket	61	1.072	7.905	12.852	0.506	3.399
Primary control	37	1.05	21.18	15.291	0.602	6.862
Secondary control	31	1.05	10.87	14.036	0.552	15.981
Reactor shield	19	1.0		25.197	0.992	1.357

The above correlations (C.17 and C.18) are provided as an option (ICORR = 94) in COMMIX.

Alternatively, one can use either of the two sets of generalized equations to determine the friction factor in fuel assemblies. In COMMIX, an additional option (ICORR \approx 90) is provided for determining the friction factor.

$$f = \frac{81.7}{Re} (1 - \chi)^{1/2} + \frac{0.48}{Re^{0.25}} \chi^{1/2}$$
 (C.20)

for CRBR fuel assemblies. Equation C.20 is derived from Eqs. C.5 and C.6 using the values P/D = 1.24 and H = 30.227 cm to evaluate the coefficient A = 81.7.

· Blanket Assembly

Engel, Markley, and Bishop³ recommended the following correlations for the blanket assembly:

$$f = \frac{99}{Re} (1 - \chi)^{1/2} + \frac{0.48}{Re^{0.25}} \chi^{1/2} . \tag{C.21}$$

Equation C.21 is provided as an option (ICORR = 91) in COMMIX.

· Control Assembly

For CRBR control assembly, if we use the generalized correlations C.5-C.7, we obtain

$$f = \frac{60.68}{Re} (1 - \chi)^{1/2} + \frac{0.48}{Re^{0.25}} \chi^{1/2}.$$
 (C.22)

Equation C.22 is provided as an option (ICORR = 95) in COMMIX for evaluating friction factor in the CRBR control assemblies.

C.2.4 Rod Bundles in EBR-II

For EBR-II rod bundles, Baumann et al. 10 used the correlation

$$f = a Re^b$$
, (C.23)

Table C.3. Important parameters of EBR-II assemblies

Assembly	No. of Rods	D, mm	P/D	H/D
Driver (fuel)	91	4.42	~1.30	3.45
Blanket	19	12.52	~1.0	- 1
Reflector	1a	-	+	**

aHexagonal cross section.

Table C.4. Values of constants a and b for EBR-II assemblies

Assembly	a	b	Range
Driver	26.33	-0.85	Re < 557.5
Driver	0.1922	-0.072	Re ≥ 557.5
Reflector	6.48	-0.03	
Blanket	2.574	-0.269	

derived from the experimental measurements. The major dimensions and the values of constants a and b for different types of assemblies are given in Tables C.3 and C.4. The constants are derived from the measurements of total pressure drop across the full length of an assembly without separating the effects of various subsections, e.g., inlet nozzle, orifice shield, rod bundle, outlet nozzle, etc. Therefore, one correlation, Eq. C.23, is applicable over the entire length of the assembly.

C.3 Spacer Grids

C.3.1 Plane Grid

For a plane grid with sharp-edged orifices (Fig. C.6), Idelchik¹¹ gave the values of loss coefficient as a function of area ratio (Table C.5):

$$\Delta p = \left(K \frac{1}{2} \rho v^2\right) n. \tag{C.24}$$

Here, n is the number of grids; K, the loss coefficient for a grid, is a function of area ratio A_0/A_1 ; A_0 is the flow area through grid; and A_1 is the flow area without grid.

C.3.2 Grid-Type Spacer

For a grid-type spacer, such as used in a rod bundle assembly, Fig. C.7, Rehme⁵ gives the following correlation:

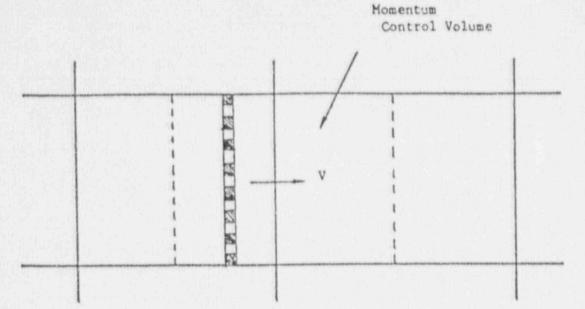


Fig. C.6. Plane grid with sharp-edged orifices

Table C.5. Loss coefficients for a plane grid

A _o /A ₁	K	A _o /A ₁	K	A _o /A ₁	К
0.02	7000	0.22	40.6	0.50	4.00
0.03	3100	0.24	32.0	0.52	3.48
0.04	1670	0.26	26.8	0.55	2.85
0.05	1050	0.28	22.3	0.60	2.00
0.06	730	0.30	18.2	0.65	1.41
0.08	400	0.32	15.6	0.70	0.97
0.10	245	0.34	13.1	0.75	0.65
0.12	165	0.36	11.6	0.80	0.42
0.14	117	0.38	9.55	0.85	0.25
0.16	86.0	0.40	8.25	0.90	0.13
0.18	65.5	0.43	6.62	0.95	0.05
0.20	51.5	0.47	4.95	1.00	0.00

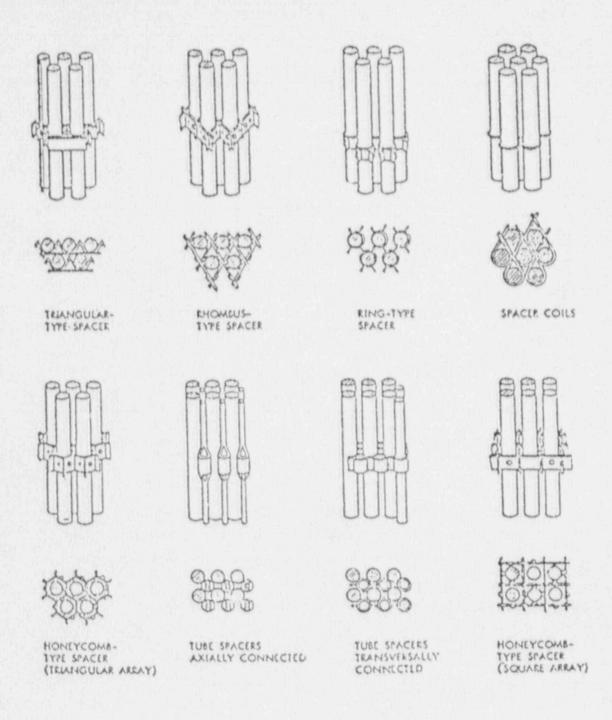


Fig. C.7. Grid-type spacers

$$\frac{\Delta p}{\frac{1}{2} p v_1^2} = K = c_v \left(1 - \frac{A_o}{A_1} \right)^2. \tag{C.25}$$

Here, the coefficient c_v has a value between 6 and 7, v_1 is the average flow velocity. A_0 is the flow area through a spacer, and A_1 is the flow area through an undisturbed section.

C.4 Crossflow in Tube or Rod Bundle

C.4.1 Generalized Correlations

For crossflow over tubes, Gunter and Shaw¹² proposed the following correlations for friction factor.

Laminar Flow (Re < 200)

$$f = \frac{\Delta p \, d_v}{L_{\frac{1}{2}} p \, v^2} = \frac{180}{Re} \left(\frac{d_v}{P_T} \right)^{0.4} \left(\frac{P_L}{P_T} \right)^{0.6} \,. \tag{C.26}$$

Turbulent Flow (Re ≥ 200)

$$f = \frac{1.92}{Re^{0.145}} \left(\frac{d_v}{P_T} \right)^{6.4} \left(\frac{P_L}{z_T} \right)^{0.6} . \tag{C.27}$$

Here,

$$d_{v} = \frac{4 \text{ x net free volume}}{\text{friction surface}}$$
 (C.28)

is the volumetric hydraulic diameter, P_L is the longitudinal pitch (center to center distance from a tube in one row to the nearest tube in the next transverse row), P_T is the transverse pitch (center to center distance from a tube to the next tube in one transverse row), and

$$R_{\epsilon} = \frac{\rho v d_{\nu}}{\mu} \tag{C.29}$$

is the Reynolds number based on volumetric hydraulic diameter.

C.4.2 Square Array

For flow across a square array, as shown in Fig. C.8, Idelchik¹¹ recommended the following correlation for pressure loss coefficient:

$$K = \frac{\Delta p_{lose}}{\frac{1}{2}\rho v^2} = (aRe^m)n. \tag{C.30}$$

Here, v is the mean velocity in the bundle cross section. Re is the Reynolds number based on mean velocity v and rod diameter D, and n is the number of transverse rows of tubes (e.g., n=3 in Fig. C.8). The coefficient a and exponent m are functions of pitch-to-diameter ratio P/D and are given in Tables C.6 and C.7.

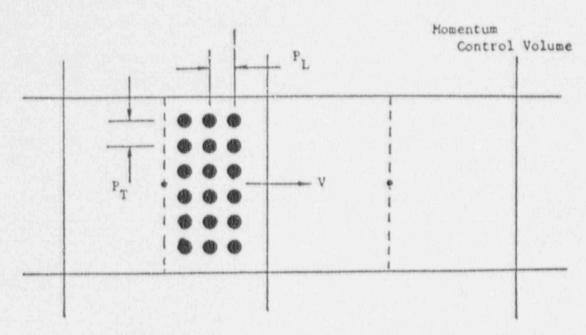


Fig. C.8. Crossflow over square array to tube or rod bundle

C.4.3 Triangular (Staggered) Rod Bundle

For flow across a staggered rod bundle, as shown in Fig. C.9, Idelchik recommended the following correlation for loss coefficient:

$$K = (a Re^{-0.27})(n+1)$$
. (C.31)

Here, Re is the Reynolds number based on mean velocity v and rod diameter D, and n is the number of transverse rows of tubes; the coefficient a is a function of pitch-to-diameter ratios and is given in Table C.8.

C.5 Sudden Enlargement and Contraction

The pressure loss due to abrupt change in area is generally expressed in terms of the loss coefficient K:

$$\Delta p = K_1 \frac{1}{2} \rho v_1^2 \tag{C.32a}$$

$$= K_2 \frac{1}{2} \rho v_2^2, \qquad (C.32b)$$

where K_1 and K_2 are the pressure loss coefficients, and v_1 and v_2 refer to the velocity in the smaller and larger cross sections, respectively.

Table C.6. Coefficient "a" for square array (Fig. C.8)

$\left(\frac{G-T_d}{G-T_d}\right)$	1.2	1.4	1.6	8,1	2.2	2.6	3.0	3.4	3.6	4.2
0.1	5.376	3.792	3.120	2.688	2.184	1.872	1.704	1.560	1.440	1.344
0,2	4.704	3.318	2.730	2,352	1.911	1.638	1.491	1,365	1.260	1.176
0.4	4.077	2.876	2.366	2.038	1.656	1,420	1.292	1,183	1.092	1.019
9.0	3.808	2.686	2.210	1.904	1.547	1.326	1.207	1.105	1.020	0.952
0.8	3,539	2.496	2,054	1.770	1,438	1.232	1.122	1.027	0.948	0.885
1.0	3,405	2.402	1.976	1.702	1.383	1.186	1.079	0.988	0.912	0.851
1.2	1,613	1,138	0.936	908-0	0.655	0.562	0.511	0.468	0.432	0.403
1.6	0.918	0.648	0.533	0.459	0.373	0,320	0.291	0.266	0.246	0.230
2.0	0.672	0.474	0.390	0.336	0.273	0.234	0.213	0.195	0.180	0.168
2.4	0.538	0.379	0.312	0.269	0.218	0.187	0.170	0.156	0.144	0.134
2.8	0.470	0.332	0.273	0.235	0.191	0.164	0.149	0.137	0.126	0.118
3.2	0,381	0,269	0.221	0.1190	0.155	0.133	0.121	0.1111	0.102	0.0952
3.6	0.336	0.237	0.195	0.168	0.137	0.117	0.107	0.0975	060.0	0.0840
0.4	0.314	0.221	0.182	0.157	0.127	0.109	0.0994	0.0910	0.040	0.0784
4.2	0.314	0.221	0.182	0.157	0.127	0.109	0.0994	0.0910	0.040	0.0784

Table C.7. Coefficient "m" for square array (Fig. C.8)

$\frac{P_T - D}{P_L - D}$	m	$\frac{P_T - D}{P_L - D}$	m
0.1	-	1.2	-0.139
0.2		1.6	-0.078
0.4	-	2.0	-0.050
0.6	-0.2	2.4	-0.0347
0.8	-	2.8	-0.0255
1.0	-	3.2	-0.0195
		3.6	-0.0154
		4.0	-0.0125
		4.2	-0.0113

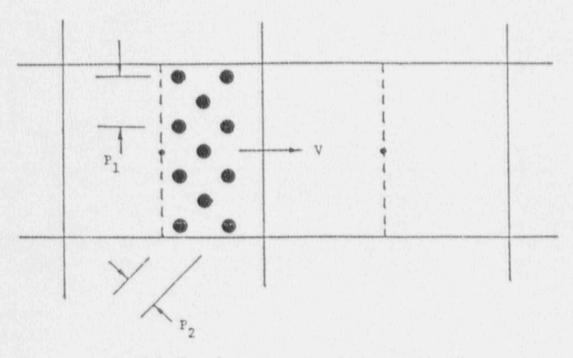


Fig. C.9. Crossflow over staggered tube or rod bundle

Table C.8. Coefficient "a" for staggered bundle (Fig. C.9)

-27	3.20	3.20		-9-	- A	79.			3					7.70	9.32	11.0	12.8	14.7	16.91
8,	. 4			3.20	1.5		1.8	3				90.6	6.34	7.70	9.32	36	12.8	14.7	6.91
3.4	3,20	3,20	3.20	3.20	3.20	3.20	3.20	3.20	3,20	3,43	3.96	5.06	6,34	7.70	9.32	0.11	12.8	14.7	16.9
3.0	3.20	3.20	3.20	3.20	3.20	3,20	3.20	3,20	3,20	3,43	3.96	5.06	6.34	7.70	9.32	0.11	12.8	14.7	16.9
2.6	3.20	3.20	3.20	3,20	3.20	3.20	3,20	3.20	3.20	3.43	3,96	5.06	6.34	7.70	9.32	11.0	12.8	14.7	16.9
2.2	3,20	3.20	3,20	3,20	3,20	3.20	3.20	3,20	3,20	3,43	3.96	5.06	6.34	7.70	9,32	11.0	12.8	14.7	16.9
11.8	4.044	4,012	3,904	3,796	3,688	3.580	3,472	3.256	3.20	3,43	3.96	2,06		7.70	9.32	11.0	. P.	- 10.7	vp.
1.6	4,889		4.608	4,392	4.176	3,960	3.744	3.312		3,43	3.96	5,06						1 4	
1.4	5.733	5.636	5.312	4.988	4.664	4.340	4,016	3,368	3,20	3,43	3.96	5.06	6.34	7.70	0.37	0 11	11 0		1.6.0
1.2	6. 578	A 848	910.9	5.584	5,152	4.720	4.288	3.424	3.20	3,43	3.96	5 D6	77. 4	7 70	0 33	1000	2 6	0.71	1.51
F 0 0 -	11.0	4 6	7*0			1.0	1 2		7	8	0.0			0.7	3.4	0.0	0.4	a	D 0

For abrupt expansion, the loss coefficient K is given by the expression 13-14

$$\mathbf{K}_1 = \left(1 - \frac{\mathbf{A}_1}{\mathbf{A}_2}\right)^2,\tag{C.33}$$

where A_1 and A_2 are the small and large areas, as shown in Fig. C.10. With the abrupt-expansion models, as shown in Fig. C.10, Eqs. C.32a and C.33 can be used directly to evaluate f and c of Eq. 6.3.

If the abrupt-expansion is modeled as in Fig. C.11, the reference velocity used in COMMIX to evaluate pressure drop now corresponds to the velocity in the larger cross section. Therefore, we must use Eq. C.32b with loss coefficient K2, given by

$$K_2 = \left(\frac{A_2}{A_1} - 1\right)^2$$
 (C.34)

For abrupt contraction, as shown in Figs. C.12 and C.13, the values of loss coefficient 15 are presented in Table C.9.

C.6 Venturi, Nozzle, and Orifice

C.6.1 Venturi

For venturi, we define the pressure loss as

$$\Delta p_{\text{looks}} = K_1 \frac{1}{2} \rho v_1^2 \tag{C.35a}$$

$$= K_2 \frac{1}{2} \rho v_2^2 \,, \tag{C.35b}$$

where K₁ and K₂ are the loss coefficients in reference to kinetic energy in the small and large cross-sections, respectively.

The loss coefficients for venturi, as shown in Figs. C.14 and C.15, can be expressed as

$$K_{1} = \left[1 - \left(\frac{A_{1}}{A_{2}}\right)^{2}\right] \left(\frac{1}{C_{V}^{2}} - 1\right) \tag{C.36}$$

and

$$K_2 = \left[\left(\frac{A_2}{A_1} \right)^2 \right] - 1 \left(\frac{1}{C_V^2} - 1 \right). \tag{C.37}$$

where the velocity coefficient c_V is a function of Reynolds number ($\rho v_1 D_1/\mu$) (Table C.10). The Reynolds number in Table C.10 is based on velocity and diameter of smaller cross sections.

Momentum Control Volume

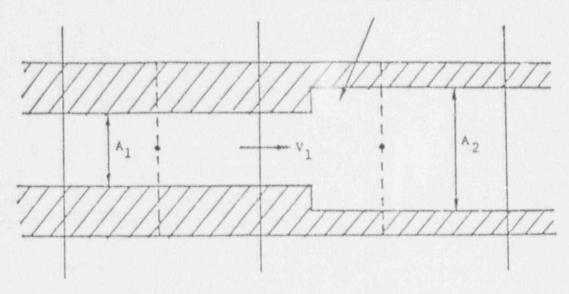


Fig. C.10. Sudden enlargement (reference velocity V_1)

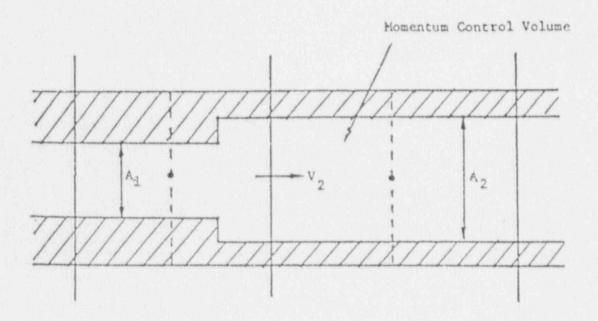


Fig. C.11. Sudden enlargement (reference velocity V2)

Momentum Control Volume

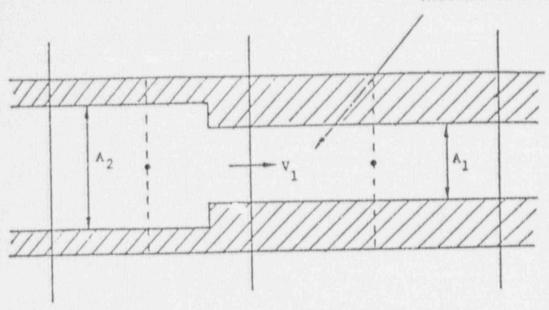


Fig. C.12. Sudden contraction (reference velocity V1)

Momentum Control Volume

Fig. C.13. Sudden contraction (reference velocity V_2)

Table C.9. Loss coefficient for sudden contraction

A ₁ /A ₂	Cc	К1	K ₂
0.1	0.624	0.363	36.375
0.2	0.632	0.339	8.475
0.3	0.643	0.308	3.422
0.4	0.659	0.268	1,675
0.5	0.681	0.219	0.876
0.6	0.712	0.164	0.456
0.7	0.755	0.105	0.214
0.8	0.813	0.053	0.083
0.9	0.892	0.015	0.019
1.0	1.0	0	0

Source: Ref. 15

C.6.2 Nozzle and Orifice

For a nozzle and orifice, as shown in Figs. C16 and C.17, we express pressure loss as

$$\Delta p = K_1 \frac{1}{2} \rho v^2 \,, \tag{C.38}$$

where

$$K = \frac{1}{C^2} \left(\frac{A_2}{A_1} \right)^2. {(C.39)}$$

Here, the discharge coefficient C is a function of area ratio and Reynolds number. The curves for the discharge coefficient of German (VDI) standard nozzles and orifice are given in Figs. C.18 and C.19.

C.7 Submerged Body

The pressure loss due to a submerged object, as shown in Fig. C.20, is given by

$$\Delta p = C_D \frac{A_p}{A_0} \left(\frac{1}{2} \rho v^2 \right). \tag{C.40}$$

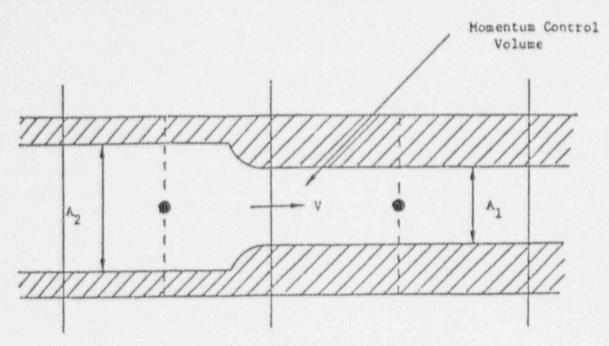


Fig. C.14. Venturi in a momentum control volume $(reference\ velocity\ V_1)$

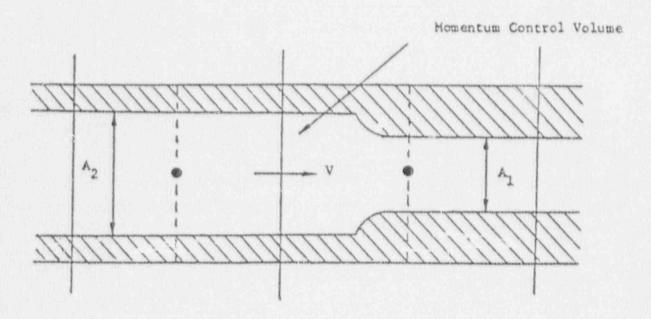


Fig. C.15. Venturi in a momentum control volume (reference velocity V_2)

Table C.10. Velocity coefficient co for venturi

Log ₁₀ Re	Cv
3.2	0.9
3.5	0.925
4.0	0.950
4.5	0.966
5.0	0.977
5.5	0.985
6.0	0.989
6.5	0.992

Source: Ref. 16.

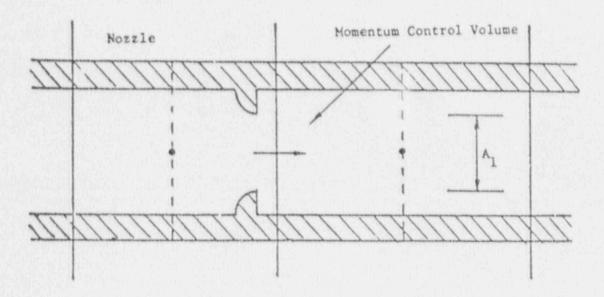


Fig. C.16. Nozzle in a momentum control volume

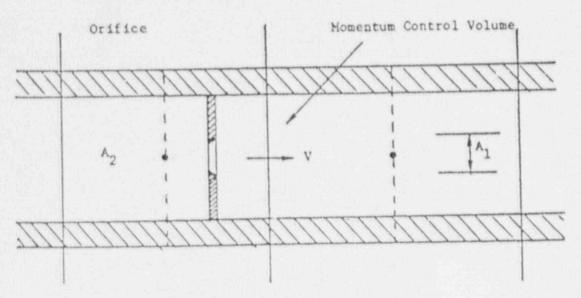
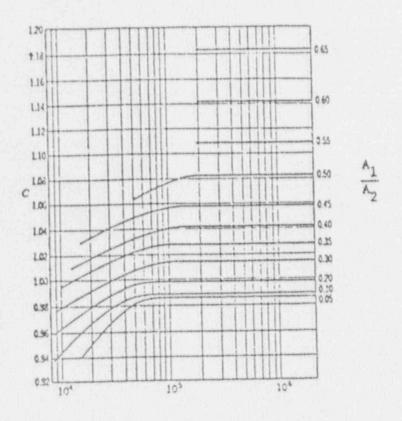


Fig. C.17. Orifice in a momentum control volume



 $Re = pv_2D_2/\mu$

A Comment

Fig. C.18. Discharge coefficient for VDI nozzle (Source: Ref. 15)

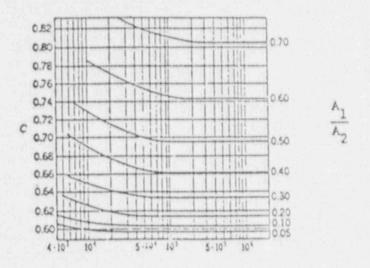


Fig. C.19. Discharge coefficient for VDI orifice

Momentum Control Volume

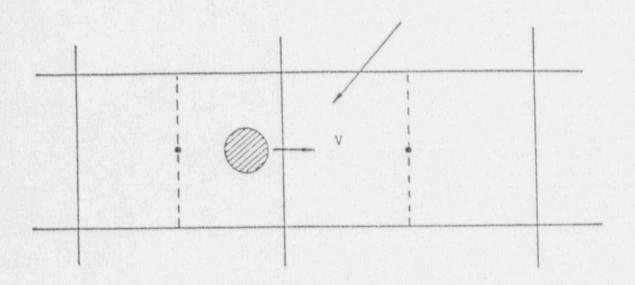


Fig. C.20. Submerged object in a momentum control volume

Here, A_p is the projected area of a submerged object, A₀ is the flow area, and C_D, the drag coefficient, is a function of Reynolds number based on velocity v and object diameter D. Figure C.21 gives the variation of C_D with Reynolds number for a few common shapes.

C.8 Porous Medium

For a packing material deposited at random, as shown in Fig. C.22, Idelchik11 recommended the following correlation:

$$\Delta p = K_1 \frac{1}{2} \rho v^2 , \qquad (C.41)$$

where

$$K = \frac{1.53}{\lambda^{4.2}} \left(\frac{\ell}{d} \right) \left[\frac{75}{0.45} \frac{(1-\lambda)\lambda^{1/2}}{Re} + \frac{15(1-\lambda)^{1/2}\lambda^{1/4}}{(0.45)^{1/2}Re^{1/2}} + 1 \right]$$

$$= \frac{\ell}{d} \left[\frac{255(1-\lambda)\lambda^{-3.7}}{Re} + \frac{34.21(1-\lambda)^{1/2}\lambda^{-5.95}}{Re^{1/2}} + \frac{1.53}{\lambda^{4.2}} \right]. \tag{C.42}$$

and

t = length of porous section.

d = average diameter of solid in porous region,

 λ = porosity (free volume fraction) in the porous region, and

 $Re = pvd/\mu$.

C.9 Straight Duct

For flow through a duct (Fig. C.23), the pressure loss is expressed as

$$\Delta p = \frac{L}{d_{\rm b}} \left(\frac{1}{2} \rho v^2 \right) f \,. \tag{C.43}$$

Here, L is the length of control volume, d_h is the hydraulic diameter, and the friction factor f is a function of Reynolds number.

· Laminar Flow

For a circular duct, the fully developed friction factor is given by

$$f = \frac{64}{Re}.$$
 (C.44)

The fully developed friction factor for a family of rectangular ducts extending from a square to flow between parallel plates is plotted in Fig. C.24. Similarly, in Figs. C.25 and C.26, the friction factors for flow between concentric annuli and a family of circular annular sectors are presented.

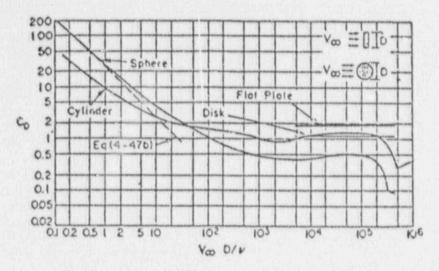


Fig. C.21. Drag coefficient for common shapes (Source: Ref. 15)

Momentum Control Volume

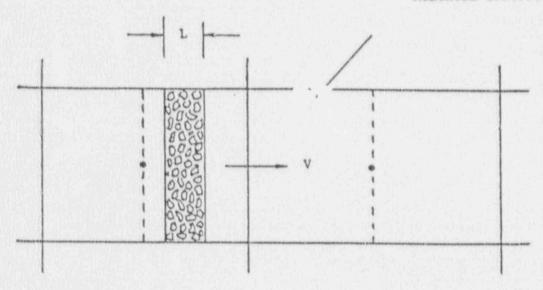


Fig. C.22. Porous medium in a momentum control volume

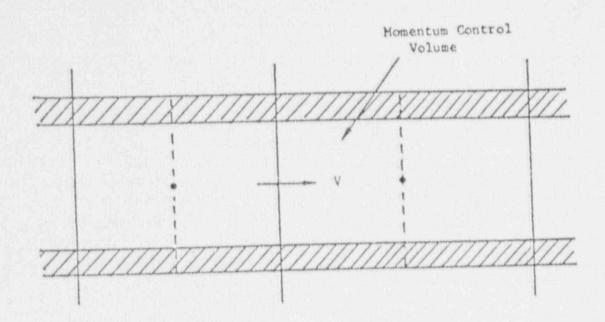


Fig. C.23. Straight duct in a momentum control volume

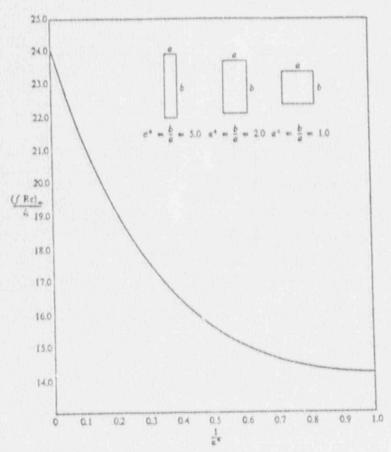


Fig. C.24. Friction factors for fully developed laminar flow in rectangular tubes (Source: Ref. 17)

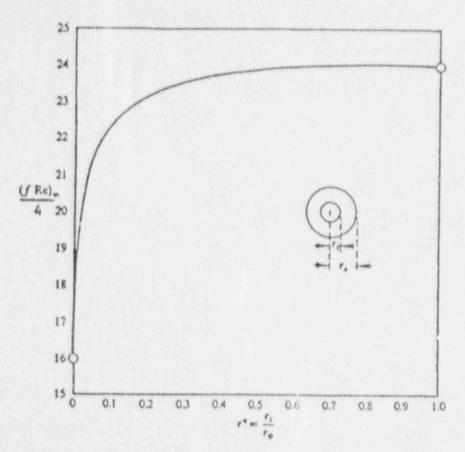


Fig. C.25. Friction factors for fully developed flow in circular tube annuli (Source: Ref. 17)

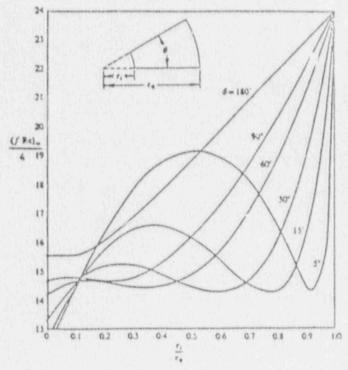


Fig. C.26. Friction factors for fully developed laminar flow in annular sector (Source: Ref. 17)

· Turbulent Flow

For turbulent flow in a straight duct, the friction factor is

$$f = \frac{0.3164}{Re^{0.26}}. (C.45)$$

Here.

$$Re = pvd_h/\mu$$
. (C.46)

C.10 Pipe Fittings

The pressure loss due to a pipe fitting is expressed as

$$\Delta p = K \frac{1}{2} \rho v^2. \tag{C.47}$$

A summary of representative head-loss coefficients, K, for typical fittings, published by the Crane Company, 18 is given in Table C.11.

C.11 Concluding Remarks

We have presented here a set of pressure loss correlations only for geometrical situations that we feel the COMMIX user is most likely to face. There are so many geometries and so many correlations that it is impossible to cover them all in this appendix. For other geometries not included here, we recommend Refs. 11, 18, and 19.

If experimental measurements are available for the geometry under consideration, it is preferable to use those data rather than a correlation from the literature.

The time spent in writing this appendix will be considered well spent if the appendix

- · Saves the user time in searching the literature.
- Prevents the user from becoming confused by so many different types and forms of possible correlations, and
- Serves as a starting reference.

Table C.11. Head loss coefficients K for various fittings

Fitting	K
Globe valve (fully open)	10.0
Angle valve (fully open)	5.0
Swing check valve (fully open)	2.5
Gate valve (fully open)	0.19
Close return bend	2.2
Standard tee	1.8
Standard elbow	0.9
Medium sweep elbow	0.75
Long sweep elbow	0.60

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Appendix D: Sample Problem 1 -Steady-State, Fully Developed, Turbulent Pipe Flow

Problem Description

Geometry:

Cylindrical pipe.

Diameter = 0.25 m.

Fluid:

Isothermal air.

Density = 1.0 kg/m^3

Viscosity = 1.5×10^{-5} Pa-s.

Reynolds No.:

5 x 105.

Mesh System:

10 (radial) x 1 (azimuthal) x 10 (axial).

Symmetry assumed in the azimuthal direction.

Flow Boundary

Inlet - uniform velocity, 30 m/s.
Outlet - continuity mass flow.

Conditions:

Pipe wall - no slip.

Pipe centerline - free slip (symmetry plane).

Thermal Bound-

Uniform temperature on all boundaries (25°C).

ary Conditions:

Pressure Bound-

Outlet pressure = 105 Pa.

ary Condition:

Other Options:

k-ε two-equation turbulence model.

Energy equation is not solved.

Pressure equation and turbulent transport equations are solved by Yale

Sparse Matrix Package.

Fully Beveloped Turbulent Pipe Flow

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outlet plane
outer wall
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Ending Address: 1037492 fd4b4
Total Storage Estimate: 1138 Kbytes

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	Total Celi Surface Area	3.663718E+02 3.663718E+02
	Surface Area In k+ Direction For All Cells	4,417875E-01 4,417875E-01
	Total Surface Area In j+ Direction For All Cells	1.250000E+01 1.250000E+0: required= 2023
	Total Surface Area In i+ Direction For All Ceils	3.534300E+02 1.25000 3.534300E+02 1.25000 = 460 space required=
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te: 7/20/90 Time: 16:57:39 C slances at time= 0.000E+00 seconds convected (Hatt) (Kg/sec) 1.877636E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.000000E+00 0.0000000E+00 0.000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.0000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.0000000E+00 0.000000E+00 0.00000E+00 0.000000E+00 0.000000E+00 0.00000E+00 0.000000E+00 0.00000E+00 0.000000E+	Global Energy Hithin Configuration: Total Internal Energy Hithin Configuration: **** Turbulent Viscosity (Pa*s) *** Turbulent Viscosity (Pa*s) *** Turbulent Kinetic Energy (J/Kg)

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COMPLIX-1C-1,1 B Last updated: 07/18/90 Nachine: 9un4/119 **********

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	60	60	10E+05	1.60E+04	ge-			0.80E+00	345	900E+		2.87E-91	185	4 4 99	

8 of time step Restart file has been written at time 8.000E+05 after iteration

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Plotting information appended to file 10.

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	Bulk Terperature (Celsius)	. 500000E+01 . 500000E+01 . 000000E+00								2. 3946- 2. 3956- 3. 7646- 7. 5436- 8. 6166- 7. 7216- 7.
								***	495 S ##	8 -8.002E-08 2.05E-08 2.05E-08 -5.129E-07 -5.129E-07 2.088E-04 1.397E-02 1.162E-02
	Average Terperature (Celsius)	2.500000E+01 2.500000E+01 2.50000E+01 9.90000E+00	(K K K K K K K K K K K K K K K K K K K	0 (kg)			6 (Joules)	***************************************	Time 8.00000E+05	7 -9 .602z -08 -2 .645z 08 -2 .645z 08 -1 .425z -05 -1 .525z -05 -1 .324z -02 -1 .324z -02
	Average Enthalpy (J/kg)	1.275025E+06 1.275025E+06 1.275025E+06 0.096090E+00	Ealarce ****** = 0.000000E+00 = 0.000000E+00	2 NF 6	= 0.000000E+00 =-4.656613E-10 = 0.000000E+00 = 0.000000E+00 = 1.592319E-06	=-1,591854E-06	= 6.258779E+106	76 10 10 10 10 10 10 10 10 10 10 10 10 10	e step 80 **	4, 013E-08 2, 358E-08 2, 358E-08 4, 759E-05 4, 535E-05 1, 359E-05
upoerted.	& D =		desset	12	dhdt hinsum qrinsum gsounc dpdt	(Apqt)	tenth	****	1 ss Time	5 4.972E 08 1.041E-07 1.041E-07 5.020E-04 5.020E-04 1.180E-03
en en	Average Velocity (h/sec)	3.000000E+01 -3.000000E+01 0.000000E+00	***************************************	11 - +1050m1	等 克 车 連 項	qinstan-qsourc-		**************************************	s* j Plane	5.266-98 5.266-98 5.496-99 1.155-98 -3.055-96 -1.457-95 4.914-94 4.914-94 5.485-94
COMMIX-1C-1.	Energy Conducted (Watt)	.000000E+00 .000000E+00 .000000E+00	· · · · · · · · · · · · · · · · · · ·	(dhasdt	**************************************	and hinsun-q		***************************************	*	3 4 0 18E - 08 4 798E - 08 4 752E - 08 - 1 135E - 05 3 139E - 05 4 248E - 04 6 052E - 04 - 8 486E - 03
16:58:43 E+85 seconds		4E + 96 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	stion :		ration :	560	figuration:	***		2.5.997E-08 4.974E-08 6.395E-08 2.051E-06 7.623E-05 3.113E-94 5.865E-05
190 Time: 16:5		1.8776 -1.8776 0.00010	Configura	Hass	e configuration Configuration		Energy Within Configurat	**********	180 (m/e)	200 - 100 -
200	, .	1,472625E+00 -1,472625E+00 0,000000E+00 0,000000E+00	**************************************	Global Conservation of Mass Total Mass Within Configurat	gy Accemulation Rate Energy Convected Into Configuration Energy Conducted Into Configuration gy Generated Hithin Configuration	Fnerdy	881	所	Walnut Walnut	
	e o	- C P	Mass Accum	Global Cont	Energy Acc Net Energy Net Energy Energy Gen	Hork Stobal Fre	Total Inte	· · · · · · · · · · · · · · · · · · ·		**************************************

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2.046E+01
1.471E+01
5.182E-02
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Appendix E: Sample Problem 2 – Steady-State, Natural Convection in a Square Cavity

Problem Description

Geometry:

2.26 cm x 2.26 cm square cavity.

Fluid:

Air (simplified properties).

Rayleigh No.:

104.

Mesh System:

20 (x) x 1 (y) x 20 (z).

Two-dimensional problem.

Flow Bound-

No slip for left, right, top, and bottom walls.

ary Conditions:

Free slip for two side walls.

Thermal Boundary Conditions: Left wall - constant temperature, 30°C. Right wall - constant temperature, 20°C.

Other walls - adiabatic.

Pressure Bound-

Pressure at upper right corner cell = 105 Pa.

ary Condition:

Other Options:

Pressure equation and scalar transport equations are solved by Yale

Sparse Matrix Package.

Steady-State Natural Convection In A Square Cavity

```
$geom
 isolvr=1, nnzere=1920, nspace=11042,
 isolve=1.
 ifres=1.
 ify=0.
 nl1=880, nm1=400,
 imax=20, jmax=1,kmax=20,
 nsurf=7.
 dx=20*1.13085e-3, dy=1.00, dz=20*1.13085e-3,
 xnorm!= 1.0,-1.0, 0.0, 0.0, 0.0, 0.0, 0.0,
 ynorm!= 0.0, 0.0, 1.0,-1.0, 0.0, 0.0, 0.0,
 znormi= 0.0, 0.0, 0.0, 0.0, 1.0,-1.0,-1.0,
 $end
                                           +x surface
                1 1
reg -1.8
             20 20 1 1 1 29 2 _x surface
1 20 1 1 1 20 3 +y surface
1 20 1 1 1 20 4 -y surface
1 20 1 1 1 5 +z surface
1 19 1 1 20 20 6 -z surface
reg -1.0
reg -1.9
reg -1.0
reg -1.0
reg -1.0
                                              -z surface
            28 20 1 1 29 20 7
reg -1.0
 &data
  idtime=0, dt=1.0e6,
  ifener=1, eps3=1.0e-6,
  it=1.
  ntmax=200, ntprnt=-9999,
  trest=1800.
  omegav=1.0, omegae=0.35,
  gravz=-9.8, temp0=25.0, pres0=1.0e5,
  kflow= 1, 1, -3, -3, 1, 1, 1,
  kpres= 6*0, 1, pres(7)=1.0e5,
  ktemp= 1, 1, 400, 400, 400, 400, 400,
  temp = 30.0, 20.0,
  veloc= 7*0.0,
  matype=1. mattab=1. tablot=20.0, tabhit=40.0,
  c0ro=1.273738, c1ro=-3.588e-3,
  c0h= 0.0, c1h=1005.7,
  c0k= 0.02624,
  c0mu=1.846e-5,
        12001,32001,52001.
  nthpr=
        12001,32001,52001,
```

send

****** Storage Allocation Variables *******

```
Variable Value <- - - - - Description - - - - ->
            8 Geometry flag
igeom
           40 Scratch space parameter
ilmax
           20 Cells in the x- or r-direction
x6mi
           0 Skew upwind flag
iskew
           1
               Energy equation solver flag
isolve
           1 Pressure equation solver flag
isolvr
          O Thermal structure flag
istruc
           O Turbulence model flag
iturke
           1 cells in the y- or theta-direction
Imax
           20 Cells in the z-direction
Kmax
          0 Number of force structures
nforce
          880 Number of surface elements
ni1
          400 Number of computational cells
nm1
         1920 Maximum number of matr.x non-zeros
nnon0
              Number of words in double precision variable
noupd
               Number of words in single precision variable
nowps
               Number of thermal structure partitions
         0
nparts
          a Number of thermal structure region's
nregts
        11042 Number of words in work space
nspace
         8 Number of thermal structures
nstruc
           7 Number of surfaces
nsurf
          0 Number of . . .
nsurts
            O Size of thermal structure storage
ntts
```

******* Sum-4/110 Truncation Error Estimate: 1.1102230246251565E-16 **********

CCMMON /SPACE/ Storage Allocated: 101569 words. (406 Kbytes) Beginning Address: 972256 ed5e0 Ending Address: 1378532 1508e4 Total Storage Estimate: 1456 Kbytes

Cells and surface elements have been counted. Check these values against your expected totals.

nm 0 Irregular computational cells
nm1 400 Computational cells (total)
nl 0 Irregular surface elements
nl1 880 Surface elements (total)

Time expended: 4.17 seconds.

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kmax= 20 dz	1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03 1,1508500E-03
7 2	5,6542500E-04 1,6962750E-03 2,8271250E-03 5,088250E-03 6,2196759E-03 7,3505250E-03 8,4813750E-03 9,6122250E-03 1,0743075E-02 1,1873925E-02 1,515455E-02 1,526475E-02 1,526475E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02 1,528175E-02
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-rex:	x 5.6542500E-04 1.6962750E-03 3.9579750E-03 5.0828250E-03 7.359250E-03 8.4813750E-03 9.6122250E-03 1.0743075E-02 1.306475E-02 1.4135625E-02 1.526475E-02 1.528175E-02 1.528175E-02 1.528175E-02
	- 200450400000000000000000000000000000000

****** Surface-Surface Element Summary *******

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Vector	0.0000 0.0000 0.0000 1.0000 1-1.0000
Unit Normal Vector	0.0000 0.0000 1.0000 -1.0000 0.0000 0.0000
E.	1.0000 6.0000 0.0000 0.0000 0.0000
Number of Surface Elements	20 20 400 400 130 130
Surface Number	
Surface Type	Regular Regular Regular Regular Regular Regular

At imp	0	Time step determination flag	alpha	1.0000E+00	
embug	0	Energy equation debug flag	dt(1)	1.0000E+06	step
fener	1	Energy equation solution flag	df(2)	1.0000E-01	Time step size after step lastdt
fmoin		Momentum equation solution flag	dtine	0.0900E+00	
- dra-	1	Restart flag	eps1	1.0000E-04	Convergence parameter
		X dimension flag	Csda -		Convergence parameter
£	u	V dimension flag	eps3	1.0000E-06	Convergence parameter
17		7 dimension flag	eps5	1.0000E-05	Convergence parameter
17.		0. carterian -1: culindrical	VCONV	1.0000E-03	par
mosk i	20		gravx	0.0000E+00	40
- Lower	2	Chair invited differenting flag	gravy	0.6000E+00	Y-component of 9, avity vector
SNOW		Hatrix colorion flag	dravz	-9.8000E+00	2-component of gravity vector
10101			Ompas	1.5000E+00	Pressure solution
state	D 6	Thousan state riay	Ombridge	7 BBBBE-01	Turbulent kinetic energy dissipation
struc	D 1	Thermal structure riag	9000000	\$ 5000F-01	Franco equation coefficients
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14(2)	10	Iterations after step lastit	onegak	A GOODE - UT	INFOUNT AMENIC SHELDS
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itibus	0		omegat	1.0000E+00	lurbulent viscosity
tmaxe	66		omega."	1.0000E+00	Under-relaxation for momentum equation
i tmaxp	66		pres8	1.0000E+05	Reference pressure
iturka	433	Turbulence model flag	rdtine	8.0000E-01	Automatic time step multiplier
Neg Y		Number of cells in y-direction	relaxe	9.5000E-01	Relaxation of energy equation solver
Comp.	20	Maximim cells in the z-direction	temp8	2.5000E+01	Reference temperature
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iestot	22777	the box of itemstions change	runt	4.2680E+00	Time spent to this point
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matype	(Code for Figure property type	404244	O DOUDE + DO	Initial simulation time
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nforce	0	Number of force structures	Squas	0.00000-00	Turkulont wineserite
nheatc	0		turby	0.0000E+00	dipolicit viscosity
n	0	Irregular surface elements	xpresu	0.0000E+00	A-, y-, and 2-
ni1	328	Number of surface elements	yp, est	B. BOCOE + OU	coordinates of the
Dim.	0	Irregular computational cells	zbres0	0 . 0000E+00	pressure reference point
run 1	400	Number of computational cells			
PSHIPF	7	Number of surfaces			

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****** Cell and Surface Element Initialization Summary *******

Variable Value I-Index J-Index K-Index Surface Number
Name Range Range Range Number of Values
Initialized

****** No cells or surface elements initialized ********

****** Cell Volume and Surface Area Summary *******

Surface	Area (m**2)
1	2.261700E-02
2	2.261700E-02
3	5.115287E-04
4	5.115287E-04
5	2.261700E-02
6	2.148615E-02
7	1.130850E-03
Total	9.149106E-02

	Yolume	Total Surface Area In i+ Direction For All Cells	Total Surface Area In j+ Direction For All Cells	Total Surface Area In k+ Direction For All Cells	Total Cell Surface Area
Total (geometric) Fluid (calculational)	5.115287E-04 5.115287E-04	4.297230E-01 4.297230E-01	0.000000E+00 0.000000E+00	4.297230E-01 4.297239E-01	8.59446 01 8.594466£ 31
giaja number of					

...gdconv... veimax= 0.000E+00 is being reset to vconv= 1.000E-03 for convergence testing.

***		Bulk Temperature (Celsius)	0000000 + 00 000000 + 00 000000 + 00 000000 + 00 000000 + 00 000000 + 00								***************************************		9 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
10 *****		m	0000,00								*	d .	8 9 000E+00 0 000E+00
Machine: Sun4/11		Average Temperature (Celsius)	3.000000E+0 2.000000E+0 2.500000E+0 2.500000E+0 2.500000E+0	*****	(kg/s) (kg/s) (kg/s)	(kg)	***	(Hatt) (Hatt) (Hatt) (Hatt)	(Haff)	(Joules)		lime U. coucou	7 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
		Average Enthalpy (J/Kg)	.017100E+04 .011400E+04 .514250E+04 .514250E+04 .514250E+04 .514250E+04	Balance *****	= 0.000000E+00 = 0.600000E+00 = 0.000000E+00	= 6.056694E-04	gy Balance ****	= 0.000000E+00 = 0.000000E+00 = 0.000000E+00 = 3.000000E+00	= 0.000000E+00	= 1,522884E+01	京東京東京 東京 東京 東京 東京 東京 東京 東京 東京 東京 東京 東京 東	step **	6 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
updated: 67/18/93			waannan	SSEH MARK	dmasdt	tmass	***** Energ	dhdt hinsum qinsum qsourc dpdt	-dpdf1	tenth	· 本 · · · · · · · · · · · · · · · · · ·	1 ** Time	0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
B Last		Average Velocity (m/sec)	0.000000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.000000E+00	*******	- flosum)		東東京東東京東京		sum-qsourc			** j Plane	000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00 000E+00
COMMIX-1C-1.1	10	Energy Conducted (Watt)	5.248000E+00 5.248000E+00 0.00000Pn:5+00 0.000000E+00 0.000000E+00	((dmasdt		- 東京在京草京京京京北京京大学 、		andt-hinsum-qinsum			In **	3 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
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Date: 7/23/90	balances at time=	Mass Convected (kg/sec)	0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00	· · · · · · · · · · · · · · · · · · ·	Hass Accumulation Rate Net Mass Convected Into Configuration Global Conservation of Mass	Total Mass Within Configuration	****	Energy Accumulation Rate Net Energy Convected Into Configuration Net Energy Conducted Into Configuration Energy Generated Within Configuration Hork	, do	Total Internal Energy Within Configurat	· 本字 · 在東京 · 東京 · 東京 · 東京 · 東京 · 東京 · 東京 · 東京 ·	vent of Velo	0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001 0,000E+001
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max(dv)/ velmax	0.00E+00 .000E+00 0.00E+00 0.00E+00	.00E+	0.006+000	0.00E+90 0.00E+90 0.00E+90 0.00E+90 0.00E+90	0.00E+00 0.00E+00 0.00E+00 0.00E+00	0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00	0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
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max(d1)/ dconv	0.00E+00 being reset 0.00E+00 0.00E+00	4 4 4 4	0.00E+00 0.00E+00 0.00E+00	00E+	0.000 0		0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
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courdt	6.25E-02	6.14E-02 6.14E-02
runt	88.57 7.88 7.88 7.73 7.88 7.73 7.88 7.73 7.88 7.73	150.32
max(dh/h)	4.77E-04 4.47E-04 4.45E-04 4.77E-04 4.45E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-04 4.77E-05 6.97E-	-1.46E-05 -1.36E-05
max(du)/	1.746.03 1.536.04 8.226.04 8.226.04 8.226.04 8.226.04 6.566.04 6.5	-5.10E-05
max(dv)/ velmax	0.00E+00 0.0	0.005+00
max(du)/ velmax	1.75E-03 1.51E-03 1.51E-03 1.51E-03 1.51E-03 1.51E-03 1.51E-03 1.51E-03 1.51E-03 1.68E-04 6.77E-05 6.77E-05 6.60E-05 6.60E-05	6.19E-05 5.71E-05
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dconv	1.94E-03 1.94E-03 1.94E-03	1.946-03	1.94E-03	1.94E-03	1.94E-03	1.946-03	1.94E-03	1.946-03	1.946-03	1.94E-03	1.94E-03	1.94E-03	1.94E-03	1.94E-83	1.94E-03	1.94E-03	1.946-03	1.94E-03	1.94E-03	1.948-03	1.94E-03	1.946-03	1.94E-03	1.94E-03	1.946-03	1 965-03	1.94E-03	1.946-03	1.946-03	1.948-03	1.946-03	1.946-03	1.775. 00
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runt	151.80 153.31 154.77 156.19	159.12	162.00	164.84	167.69	170.50	173.36	174.79	177.64	179.06	181.89	183.34	184.76	187.61	189.04	190.50	193,34	194.79	196.21	199.05	200.56	201.98	204.82	206.25	207.71	210 54	211.98	213.39	214.81	216.29	219.18	220.71	CCC- 11
max(dh/h)	-1.26E-05 -1.17E-05 -1.09E-05	-9.40E-06 -8.75E-06 -8.13E-06	-7.56E-06 -7.03E-06	-6.08E-06	-5.66E-06	-4.90E-06	X 3		-3.43E-06	T	1 1	7	-2.42E-06	1 1	T.	-1.83E-06	-1.60E-06	-1.48E-06	-1.39E-86	-1.27E-06	-1.13E-06	-1.06E-06	-9.25E-07	1	-8.08E-07	7 045-07	-6.56E-07	-6.17E-07	-5.73E-07	-5.40E-07	-4.73E-07	-4.38E-07	10 THE OF
max(da)/	-4.41E-05 -4.16E-05 -3.82E-05 -3.60E-05	-3.31E-05 -3.12E-05 -2.87E-05	-2.70E-05	-2.34E-05 -2.16E-05	-2.03E-05	-1.76E-05	1 1	T	-1.236-05	1.16E-	-1.08E-05	38E-	-36E-	- 2	1		-5 885-06	1	. 15E-	1	-27E-	-3.98E-06	-3.75E-06	T		-2.94E-UB	-2.60E-06			-2.15E-06	-1.91E-06	-1.84E-06	1.7 15 00
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Plotting information appended to file 10.

	ulk enperature Celsius)	10E+00 10E+00 10E+00 10E+00 10E+00 10E+00								* * * * * * * * * * * * * * * * * * *		5.328E-03 1.175E-02 1.484E-02 1.557E-02 1.293E-02 1.710E-03 7.710E-03 7.710E-03 7.710E-03 7.689E-03 1.563E-03 1.563E-03 1.564E
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nacrine-sume	Average Temperature (Celsius)	3.000000E+01 2.009383E+01 2.09388E+01 2.2.069E+01 2.739.9E+01 2.739.9E+01	****	(kg/s) (kg/s) (kg/s)	(kg)	*****	(Watt) (Matt) (Matt) (Watt)	(Hatt)	(Joules)	* 600		5.231E-03 5 1.108E-02 1 1.36E-02 1 1.316E-02 1 1.316E-02 1 1.316E-02 1 2.679E-03 7 4.477E-03 4 1.594E-03 1 1.594E-03 1 1.594E-03 1 1.594E-03 1 1.594E-03 1 1.571E-02 1 1.351E-02 1
077 107 70	Average Enthalpy (J/kg)	.017100E+04 .011400E+04 .513634E+04 .513634E+04 .305134E+04 .754772E+04	Balance *****	3.294794E-20 0.000000E+00 3.294794E-20	6.056806E-04	Balance ***	-4.996354E-15 0.000000E+00 -4.820615E-08 0.000000E+00	4.820615E-08	1.521225E+01	** ** **	and done	6 4.907E-03 1.017E-02 1.279E-02 1.279E-02 1.279E-03 6.796E-03 4.367E-03 1.750E-03 1.75
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COMMIX-1C-1.1	Energy Conducted (Watt)	.097302E-01 .097302E-01 .000000E+00 .000000E+00 .000000E+00	*********	(dnasdt		**********		andt-hinsum-qinsum			in **	2.420E-03 4.881E-03 5.881E-03 6.105E-03 8.105E-03 6.105E-03 7.13E-03
Time: 16:14:24 1.610E+08 seconds		.000000E+00	** ** ** ** ** ** ** ** ** ** ** ** **	rtion :		***********	ration :	16	iguration:	本本 本本 本本 本本 本本 本本 本本 本本 本 本 本 本 本 本 本		2. 691E-03 3.269E-03 3.269E-03 3.413E-03 3.194E-03 2.929E-03 2.929E-03 2.980E-03 1.790E-04 4.157E-05 -9.630E-04 -1.939E-03 -2.915E-03
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Date: 7/23/90 balances at time=	Mass Convected (kg/sec)	0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00	********	Mass Accumulation Rate Net Mass Convected Into Configuration Global Conservation of Mass	Within Configuration	京京市大学大学大学大学大学	Energy Accumulation Rate Net Energy Convected Into Configuration Net Energy Conducted Into Configuration Energy Generated Within Configuration Rork	797	otal Internal Energy Within Configurat		nent of Velocity	0.000E+00) 3 0.000E+00) 3 0.000E+00) 3 0.000E+00) 3 0.000E+00) 3 0.000E+00) 4 0.000E+00) 4 0.000E+00) 4 0.000E+00) 4 0.000E+00) 4 0.000E+00) 4 0.000E+00) 4
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