APR 1 3 1981

MEMORANDUM FOR: Harold Denton, Director
Office of Nuclear Reactor Regulation

FROM: Robert B. Minogue, Director
Office of Nuclear Regulatory Research

SUBJECT: RESEARCH INFORMATION LETTER #120
APPLICATIONS OF THE COMMIX
3-DIMENSIONAL THERMAL HYDRAULIC COMPUTER CODES

1. Introduction

This Research Information Letter (RIL) describes the COMMIX (Component Mixing) family of computer codes and discusses some of the applications of these codes. Since there has been no licensing activity on Liquid Metal Fast Breeder Reactors by NRC in the past several years, there has been only nominal interest in the NRC (outside RES) in the Three-Dimensional Transient Thermal Hydraulic Computer Code Development Program at the Argonne National Laboratory. Nevertheless the program to develop COMMIX codes has been continued to provide a tool for licensing LMFBR's in the future. In addition, the code has been applied to a wide variety of LWR design problems.

The initial objective of the Argonne National Laboratory Program, "Three-Dimensional Code Development for Core Thermal Hydraulic Analysis of LMFBR Accidents Under Natural Convection," was to develop a benchmark code for the detailed study of natural convective heat removal in an LMFBR during a loss of forced circulation accident. The original version of the code COMMIX-1[1] was slow running and was useful only to solve benchmark problems at great computer expense (hours on an IBM 195). Since that version, improvements have been made in the numerics[2] of the code and in the initialization scheme so that COMMIX 1A, running more than 10 times faster than COMMIX-1, is a practical code for solving engineering problems. The two-phase version of the code COMMIX-2 is operational and has been documented.[3] The code has improved numerics[4] over COMMIX-1A which makes transient two-phase flow calculations feasible. In order to analyse experimental data in an endeavor to obtain better sodium boiling models for COMMIX-2, a specialized code BODYFIT-IFE[5,6,7] has been developed to analyse small hexagonal fuel-rod bundle without the usual subchannel analysis assumptions. Although COMMIX was developed to be a research tool, it has developed into a tool that should be useful when licensing of Clinch River Breeder Reactor resumes.

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Since the COMMIX code is well documented and the primary purpose of
this RIL is to discuss application, the details of the code structure
will not be discussed here. An excerpt from the COMMIX-2 code des-
cription [3] is enclosed. References 1-8 give descriptions of
the models and individual computer codes.

As the improvements have been made in the COMMIX codes and the use-
fulness of some of its features such as volume porosity, surface per-
meability have been understood, the code has been widely accepted by
the LMFBR community. The computer program has been obtained by nearly
all of the organizations, domestic and foreign, that are working
on LMFBR technology. The codes have also been applied to high temp-
erature gas cooled reactors and LWR component problems.

2. Results

Five applications of COMMIX-1A are reported in a paper by H. M. Domanus
et al. [9,10]. These applications use the porous medium approach.
The experiments studied are referenced in the reports. The appli-
cations are:

(a) Natural circulation in a 19-pin bundle with a 3:1 radial
power skew. As shown in Figure 4 of the paper, the agree-
ment between measured and calculated outlet temperature dis-
tribution is excellent.

(b) Planar blockage in a 19-pin bundle. As shown on Figure 17
of the paper, the agreement between calculated outlet tempera-
ture is within 5^0C. A wire wrap force treatment is necessary
to obtain reasonable agreement at the wall.

(c) Loss of piping integrity transient in a 19-pin bundle.
This is a rapid flow and power reduction transient. As
shown in Figures 21 through 24 of the paper, the agreement
between measured and calculated temperatures vs time is good.

(d) Flow rundown in a seven pin bundle. This is the German
7-pin flow rundown experiment without rundown of power until
boiling starts. The calculated time to incipient boiling
assuming the measured 68^0C superheat condition is 6.28s
which compares favorably with the measured 6.37s. As shown
on Figures 28 through 32, the agreement between measured and
calculated temperatures vs time in the bundle is excellent up
to the point where the sodium becomes superheated. This
experiment was also calculated using the BODY-IFE code with
good agreement [11].

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    (e) CRBR outlet plenum transient in a 1/10 scale flow model.
This is an example of COMMIX's ability to handle a complicated
three dimensional geometry. As shown on Figure 41 of the
paper, the agreement between measured and calculated tempera-
tures vs time at the exit and at the top of the plenum is
good. The relatively poor agreement during part of the transient
at thermocouple (TC) 12 is due to the coarse mesh used in
the calculation. As shown in Figures 27-38 a stratified layer
formed at TC12. The code was calculating the average tempera-
ture of a 20 cm thick region, while the thermocouple was meas-
uring the temperature above the stratified layer.

A simulation of a flow and temperature transient in an intermediate
pipe loop during a typical CRBR scram, calculated using the COMMIX-1A
code, is reported in reference 12. Because of the parabolic inlet
velocity distribution and the temperature decrease at the inlet, cooler
sodium penetrates into the central portion of the pipe and is relatively
cooler than the bottom portion early in the transient. As a result of
the flow redistribution, a considerable top to bottom temperature difference
(in excess of $65^{\circ}C$) due to flow stratification was found in the later
part of the transient. Temperature gradients of this magnitude need
to be considered in evaluating piping integrity.

Some early results using COMMIX-2 are reported in reference 13.
These are:

    (a) Transient single-phase flow with heat flux.

    (b) Two-phase flow with heat flux from a wall.

    (c) Separation of vapor and liquid by gravity forces.

    (d) High-pressure jet impingement on a vertical wall.

The reported results confirm the ability of COMMIX-2 to handle transient,
three-dimensional, two-phase flow.

Application by non-NRC users

The COMMIX-1A computer code has been obtained by 14 non-NRC users.
Although they are not adequately documented to be referenced in this
RIL, there are a number of user applications of the code that may be
useful within NRC.

    (a) A version of the code COMMIX-IHX has been developed by
Foster Wheeler and ANL for analysis of intermediate (sodium
to sodium) heat exchangers under DOE sponsorship.

    (b) Westinghouse (WARD), General Electric, and Babcock & Wilcox
Co. are using the code to analyze flow patterns in LMFBR plena.

    (c) The flow pattern in the Donnreay PFR reactor vessel is being
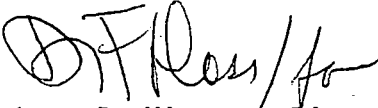analyzed at ANL under the current NRC program in accord with
ACRS recommendations.

(d) General Atomics Co. has used the code to analyze natural convection in upper plenum of the HTGR during loss of forced flow conditions. They have also used it to analyze the natural convection in the core, upper plenum and lower plenum of the gas cooled fast reactor in a single calculation (see enclosure 2).

(e) ANL is setting up a complete in vessel calculation for a pot-type LMFBR as a carry-on of the Conceptual Design Study.

(f) The Westinghouse Electric Corporation Steam Generator Division and ANL have made a joint proposal to DOE to develop and verify steam generator codes based on the COMMIX codes. The code would be used to analyze flow patterns, temperature transients, and vibratory forces.

3. Evaluation

The COMMIX-1A code has been well tested against experimental data on sodium and water systems and can be used with confidence to evaluate transient flow patterns, temperature distributions and flow-induced forces in fuel-rod bundles and reactor components where single-phase flow is applicable. The code has been used by General Atomic Company on helium systems. They are enthusiastic about the code but have not done any appreciable testing against experiment. A scaled plenum flow experiment is planned but is several years away. Further evaluation of the code against experiment is recommended before relying on it for assessment of gas cooled reactors.

COMMIX-2, the two phase version of the code, is applicable to transient dispersed turbulent flow. Unfortunately, results are sensitive to the drag coefficient (K) and evaporation-condensation rate constants, as are all two-phase flow computer codes. Also, more work is needed on initiation of boiling models since the degree of superheat before initiation of boiling is unpredictable in sodium systems. A comparison between COMMIX and other thermal hydraulic codes (TH13D-1, COBRA-111C, and SABRE-1) is given in reference 14.

RES contact:
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Enclosures: As stated
1. Excerpt from COMMIX-2 Report
2. Letter 2/17/81, Del Bene, GA to Kelber, NRC

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T. Speis, NRR
G. W. Knighton, NRR
R. Audette, NRR
P. Williams, NRR
B. Sheron, NRR

References:

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2. V. L. Shah, et al. "A Numerical Procedure For Calculating Steady/Unsteady, Single-Phase/Two-Phase Three-Dimensional Fluid Flow With Heat Transfer," NUREG/CR-0782, ANL-CT-79-31, June 1979.

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13. V. L. Shah, et al. "Some Numerical Results With the COMMIX-2 Computer Code" NUREG/CR-0741, ANL-CT-30, March 1979.

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I.   INTRODUCTION

The present-generation computer speed and storage capacity, coupled with recent advances in numerical-solution techniques for systems of quasi-linear partial differential equations, have made possible detailed numerical simulation of many engineering problems. With the anticipated improved performance of the next generation of computers and further advances in numerical-solution techniques, use of numerical simulation for solving engineering problems is expected to increase for many years to come.

Basically, numerical simulation in engineering applications can be classified into two categories: the system computer program and the component computer program. Generally, the system computer program consists of a number of components; therefore, it cannot afford to give a detailed numerical modeling of each component. In contrast, the component computer program deals with one component of interest; therefore, it can afford to provide a detailed numerical simulation. The work presented in this report is focused on the component computer program.

During loss of coolant or transient overpower accident situations, boiling of liquid coolant in a reactor core is postulated due to high temperatures in the core. The fluid mixture of liquid and vapor, in such circumstances, is nonhomogeneous with both phases being in nonequilibrium thermodynamic states. It is, therefore, desirable to develop a computer code for obtaining numerical solutions of three-dimensional, transient, two-phase (gas-liquid) flow system with nonequilibrium and nonhomogeneous conditions.

The COMMIX-2 code is a steady/unsteady, three-dimensional two-phase computer code for thermal hydraulic analysis of reactor components under normal and off-normal operating conditions. It uses the two-fluid model of Harlow and Amsden.[5] to describe the conservation equations of mass, momentum and energy. Consequently, we can analyze a wide spectrum of flow conditions; i.e., from homogeneous and equilibrium to nonhomogeneous and nonequilibrium condition. The interactions between two fluids are accounted for by incorporating the corresponding terms in all of the conservation equations. The staggered grid system is used to describe the field variables at the center of a cell and flow variables at the center of a cell and flow variables at the surface of a cell.

The structure of the code is similar to that of COMMIX-IA.[2] The calculation procedure employed is an extension of the single-phase numerical procedure,[16] known as SIMPLER (Semi-Implicit Method for Pressure Linked Equation-Revised). In this procedure, we use the liquid phase continuity equation to obtain the void fractions, and use the combined continuity equation to derive the pressure and pressure correction equations.

The specific features of COMMIX-2 are the following:

1. To permit an analysis of a flow domain with solid objects, the volume porosity, surface permeability, distributed resistance and distributed heat source are incorporated in the conservation equations.

2. An approximate form of Spalding's equation[17] is used to derive the the finite difference formulation of the convective and diffusion terms. This equation is a function of the Peclet number and it combines the best features of both, the central difference and upwind difference schemes.

3. The discretization equations are obtained by integrating the conservation equations over a control volume surrounding a grid point. Thus, the Derivation process and the resulting equations have direct physical meaning, and the consequent solution satisfies the conservation principles.

4. The convective, diffusion, interfacial friction and interfacial heat transfer terms are made implicit for more stable formulation and to permit larger time steps.

5. The discretization equations are formulated with time step size appearing only in the denominator of all transient terms. With this arrangement, for a steady state calculation, all of the transient terms can be eliminated from computation by specifying a very large value of time step size.

6. The general form of all discretization equations is

$$a_0 \phi_0 + \sum_{nb} a_{nb} \phi_{nb} = b_0,$$

where, ϕ is a dependent variable and subscript NB stands for neighboring points. This general form of the discretization equation permits various solution schemes, e.g., cell by cell, line by line, plane by plane, block iterative, direct inversion etc.

7. The COMMIX-2 code is structured such as to permit solution of single phase (gas or liquid) as well as two-phase (gas and liquid) flow problems. In addition, it permits 1D, 2D, or 3D calculation in either (X,Y,Z) or (R,Z,Θ)coordinates.

8. The COMMIX-2 code has modular structure. This permits rapid implementation of the latest available drag models, heat transfer models, boiling models, etc.

9. The code has also an option permitting use of either sodium property package or water property package.

10. The program also contains
    (i) A generalized resistance model to permit determination of resistance due to internal structures (fuel rods, wire wrap, baffles, grid spacers, etc.)

(ii) A generalized thermal structure formulation to model thermal interaction between structures (fuel rods, wire wraps, duct wall, baffles, etc.) and surrounding fluid, and

(iii) A local regional mass rebalancing scheme, such as plane by plant, for improving the convergence rate.

This report describes the COMMIX-2 program for the solution of the governing equations for three-dimensional, single-phase/two-phase, steady/unsteady flow with heat transfer. The description here starts with the differential equations and deals with numerical method incorporated into a computer program. Section 2 is devoted to the set of governing equations for the situation considered. In Subsection 2.4, the general form of all the governing equations is recognized; this generalization facilitates a unified development of the numerical method and the construction of the computer program.
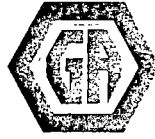
The conservation equations for quasi-continuum regime are presented in Section 3. We define the quasi-continuum regime as a medium which contains finite, dispersed, stationary heat generating (or absorbing) solid objects. The effects of solid objects in a medium are accounted for by introducing volume porosity surface permeabilities, distributed heat sources. The physical models and constitutive equations used in COMMIX-2 for describing the mass, momentum and energy exchange phenomena are presented in Section 4.

In Section 5 we present some preliminary considerations before we start assembling the finite difference equations. The finite difference equations. The finite difference formulation of the general equation is presented in Section 6. As we use a staggered grid system, the control volumes for momentum equations are different and require special considerations. The special features of the finite-difference equations for momentum are discussed in Section 7. In Section 8 we have presented the finite difference forms of the continuity equations.

Section 9 contains the derivation of pressure and pressure correction equations. In the present program we have two alternative forms of pressure correction equation leading to two alternative solution procedures. The first procedure is an extension of the single-phase numerical procedure,[16] known as SIMPLER (Semi-Implicit Method for Pressure Linked Equation-Revised). In this procedure we use one of the two phase continuity equations to determine the liquid volume fractions, and use the conbined continuity equation to derive the pressure correction equation. In the second procedure we use both of the phase continuity equations to determine the liquid volume fractions; the difference lies in the derivation of the pressure correction equation. In this procedure we differentiate the phase continuity equations and momentum equations and then combine them to obtain the pressure[18] known as Inter Phase Slip Analyzer (IPSA).

Section 10 deals with the boundary conditions for the different dependent variables. A discussion of the ways of handling irregular geometries is included in Subsection 10.4. A line-by-line procedure for solving the finite-difference equations is presented in Section 11. For most of the problems analyzed, this procedure has been found to be superior to the usual point-by-point procedure without rebalance technique. In Section 12, we take an overall view of the entire calculation sequence. The various steps in the iteration scheme are listed in Section 12.1, while the remainder of Section 12 is devoted to matters that enhance the chances of obtaining a converged solution. Section 13 describes the flow chart.

The thermodynamic and transport properties of sodium and water are given in Appendix A. The thermal structure module is described in Appendix B. Appendix C contains the descriptions of the resistance and wire wrap models. The code input description and sample problems are given in Appendices D and E, respectively.

GENERAL ATOMIC

February 17, 1981

Dr. N. Kelber, Assistant Director
Advanced Reactor Safety Technology
Office of Reactor Safety Research
United States Nuclear Regulatory Commission
Washington, D.C. 20555

Dear Dr. Kelber,

This letter supports the development of the COMMIX computer program at Argonne National Laboratory.
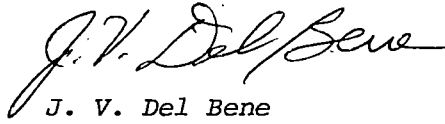
In early 1979 I requested from your office via Dr. P. M. Wood permission to get a copy of the COMMIX computer program at General Atomic Company. This request was granted, and we received a copy of the code from Dr. W. T. Sha at ANL. After a slight modification of the code to accept helium properties, we used the code for the analysis of flow and pressure drop in the lower plenum of the high temperature gas cooled reactor (HTGR). In early 1980 we requested and received the updated COMMIX-1A version. We have used this version to analyze the natural convection in the upper plenum of the HTGR and the overall natural circulation in the core, upper plenum and lower plenum of the helium cooled breeder reactor (the GCFR). Both of these analyses were for loss of forced coolant accidents. Currently, we are updating our original HTGR lower plenum model and we are developing a COMMIX-1A model of a helium-to-water helical coiled steam generator.

Our use at General Atomic Company has been exclusively with the general geometry option, the so-called box geometry, since this option allows a variety of application. With this option we can foresee other future applications; for example, flow in our HTGR fibrous insulation and flow through crushed rock in an oil shale study.

We appreciate your support of the COMMIX code, and we encourage
further support of its development at ANL. The people in the
Components Technology Division at ANL, especially Dr. H. Domanus,
have been very helpful to us at General Atomic as we have gradually
come to learn and use the COMMIX code. Thank you again.

Sincerely,

J. V. Del Bene
Systems Analysis Branch

JVDB:sc

cc: Dr. W. T. Sha,
     Argonne National Laboratory

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(d) General Atomics Co. has used the code to analyze natural convection in upper plenum of the HTGR during loss of forced flow conditions. They have also used it to analyze the natural convection in the core, upper plenum and lower plenum of the gas cooled fast reactor in a single calculation (see enclosure 2).

(e) ANL is setting up a complete in vessel calculation for a pot-type LMFBR as a carry-on of the Conceptual Design Study.

(f) The Westinghouse Electric Corporation Steam Generator Division and ANL have made a joint proposal to DOE to develop and verify steam generator codes based on the COMMIX codes. The code would be used to analyze flow patterns, temperature transients, and vibratory forces.

3. Evaluation

The COMMIX-1A code has been well tested against experimental data on sodium and water systems and can be used with confidence to evaluate transient flow patterns, temperature distributions and flow-induced forces in fuel-rod bundles and reactor components where single-phase flow is applicable. The code has been used by General Atomic Company on helium systems. They are enthusiastic about the code but have not done any appreciable testing against experiment. A scaled plenum flow experiment is planned but is several years away. Further evaluation of the code against experiment is recommended before relying on it for assessment of gas cooled reactors.

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Original Signed By

Benwood F. Ross, Jr.
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RES:D
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SURNAME ►	PWOOD:de	CURTIS	KELBER	BASSETT	V.L.	ROSS
DATE ►	3/26/81	3/26/81	3/27/81	4/1/81	4/16/81	4/ /81

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