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DOE/MC/19265-1479
(DE84000446)

RECOMMENDED DOCUMENTATION PLAN FOR THE FLAG AND CHEMFLUB COMPUTER CODES

By
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September 2, 1983

Work Performed Under Contract No. AC21-82MC19265

For
Morgantown Energy Technology Center
Morgantown, West Virginia

By
The BDM Corporation
Houston, Texas

and

Exxon Research and Engineering Company
Baytown, Texas

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Printed in the United States of America
USDOE Technical Information Center, Oak Ridge, Tennessee

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Distribution Category UC-90c

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FOREWORD

This technical report, BDM/A-83-017-TR, entitled "Recommended Documentation Plan for the FLAG and CHEMFLUB Computer Codes", is submitted to the Morgantown Energy Technology Center as required under Contract Number DE-AC21-82MC19265, "Testing, Evaluation, and Validation of Detailed Mechanistic Computer Codes for Fluidized Bed Gasifiers". This summary document is provided as an interim response to task 3.2, "Review and Documentation of the Models and Codes".

TABLE OF CONTENTS

I. EXECUTIVE SUMMARY

A. OVERVIEW

Reviews have been conducted on both FLAG and CHEMFLUB's documentation and computer codes. The documentation of both models is: (1) incomplete, (2) confusing, (3) not helpful to the reader, (4) filled with extraneous information and (5) lack claimed versatility in analyzing coal gasifier systems. The documentation is such that the computer coding itself must be used as a reference to complete the documentation.

Once the codes are set up they are relatively easy to run. We have exercised both of them. Most of our efforts thus far have been concentrated on FLAG because of its importance and complexity. FLAG in its present form can not be expected to yield meaningful data applicable to coal gasifier systems. The reasons for this are twofold. First, the model is incorrect in describing some aspects of fluid particle behavior in coal gasifier systems. Second, the numerical formulation/solution methodology is incorrectly implemented and introduces spurious numerical effects, thereby obscuring the physics of the model. In brief, this means that resulting calculations are not correctly related to the physics. CHEMFLUB, while less extensively exercised, shows that it should be no surprise that CHEMFLUB is best utilized as a tool for generating first approximations.

We have concluded from these reviews that we cannot perform meaningful comparisons as required under tasks 3.3, 3.4, and 3.5 without first reconstructing and correcting when necessary the physical/numerical models. A plan is presented for accomplishing this reconstruction/modification.

The possibility exists, however, that the problems to be encountered in evolving the present codes into usable coal gasifier tools may be of such a magnitude to warrant adapting an accepted time dependent, reacting fluid code and extending this code to incorporate the full physics and chemistry associated with coal gasifier systems.

B. HIGHLIGHTS OF FINDINGS

In FLAG, regarding the fluid equations (see blue tab):

- The documentation does not present the energy equation in a fully conserved form, (the present formulation can lead to instabilities in the flow field).
- The model is incorrect for modeling low or high Reynold's number flows.
- The model ignores bulk viscosity and all terms related to flow compressibility in the momentum equation.
- The documentation lacks description of initial and boundary conditions.

In the physical formulation of the fluid/particle chemistry (see blue tab):

- The chemistry model does not treat any homogeneous kinetics processes.
- CH_4 kinetics is ignored, for example, $C + 2\ H_2 \rightarrow CH_4$.
- The assumption of instantaneous devolatization is too elementary.
- The char/oxygen reaction restricts modeling to low temperature operation.

Examination of the closure equations show that (see blue tab):

- Laminar mixing is ignored in the documentation, although included in the code.

- When the code is exercised in the laminar regime, highly diffusive effects are seen that are totally inconsistent with laminar theory.

- The code does not correctly predict even simple flow in a pipe. The calculated velocity flow field is incorrect.

- Numerical effects are inducing large artificial diffusive effects into the problem.

- Computer runs to study the effects of mixing in a configuration of concentric jets in a pipe show no variation with turbulent mixing length.

- Severe numerical problems are indicated by runs in which large diffusive effects are seen with all physical diffusional quantities set equal to zero.

In the solution algorithms reviews (see blue tab):

- Exercising of the code shows that for large time steps (on the order of the fluid-convective time) the number of iterations required for convergence is not consistent with the documentation. This indicates improper implementation of the numerical scheme.

The principal problem of CHEMFLUB is the complete lack of documentation for numerical techniques. The implication of this is that all numerical issues must be addressed via a line by line examination of the computer code. This is extremely undesirable due to the inefficiency of this method to obtain information which should be in the existing documentation.

C. RECOMMENDATIONS

We include in this document our plans for reconstructing the documentation from the codes over the next 4 month period. The reconstruction step is essential for the completion of tasks 3.3, 3.4 and 3.5. We also have layed out the structure we will provide for the final documentation due in 18 months. The final documentation will consist of 3 volumes of each code: a technical volume, a user's manual and a systems manual. The systems document will be oriented towards the systems analyst who wishes to modify the codes. The other volumes will be written for an applications oriented user.

D. COMMUNICATIONS

The reconstruction of these codes will be difficult and will demand careful attention from our technical staff. We strongly advise that close technical links be established between the BDM-Exxon technical team and their counterparts at DOE on two-levels. First, DOE staff should come to our Albuquerque computer center and spend some time working with our people and second, METC should link to the BDM-VAX in Washington, D.C. to facilitate the monthly transfer of modified codes.

E. STRUCTURE OF THE REPORT

FLAG and CHEMFLUB are discussed in separate chapters. Each chapters begins with general comments (Section A) on the findings. Next comes the recommended outline (Section B) for the final documentation. These are the same for both codes, but are repeated in each chapter because the subsequent discussions of the individual codes are different.

Section C is a discussion of the principal outline sections. The section begins with a table relating major outline sections to the existing documentation and the actions required. This table, as suggested in our proposal, describes the existing documentations simply in terms of whether or not it is: (1) acceptable, (2) inadequate, or (3) not available. A detailed description of each major outline element follows the table. Each description:

(1) States the purpose and content of the outline element.

(2) Describes the status of the existing documentation and code.

(3) Describes the actions to be taken.

The recommended plan is described in Section D. This plan discusses reconstruction of the documentation, the schedule for delivery of final documentation and the communication and logging of modifications.

CHAPTER II
FLAG

A. GENERAL COMMENTS

The FLAG code has been exercised and its documentation checked. Sections of the code will run (fluids, chemistry, particles) and will provide output data. However, major discrepancies have been found between the code and the documentation and it appears there are basic problems in the numerical solution algorithms. We have also found the documentation incomplete, hard to follow and useless for identifying problems found in the code output. Therefore, our documentation plan includes an initial step of reconstructing the documentation.

The reconstruction is necessary because accurately defined equations and solution algorithms are necessary to allow output errors or strange behavior to be traced. This reconstruction will proceed by a line by line examination of the code and by exercising specific code sections.

The documentation of the JAYCOR FLAG computer code has not been presented in a manner which assists the reader in following the logic used in the development of the computer model. In fact, the presentation is confusing, hard to follow and contains internal inconsistencies. Considerable technical detail has been incorporated in the technical report. However, a large amount of this detail could be eliminated. For example, considerable effort is expended in the development of the basic conservation equations of fluids. Any standard reference could be cited. The technical report need only include the final equations. As a second example, considerable effort is expended discussing technical issues which are not part of FLAG and consequently should not be included in the FLAG report, (e.g., Vol. I Appendix B of JAYCOR's Final Report).

More fundamentally, the sequencing of the sections of the report also does not assist the reader in smoothly and coherently following the evolution of the computer code from the statement of the theory and basic equations through the operation of the code. FLAG uses an extremely spohisticated model of fluid-particle flow. Much greater care than is demonstrated in the existing documentation must be exercised in walking the reader through all the theory.

This same concern exists in the formulation of the differencing forms and solution algorithms. Insufficient details are presented in these areas. They need to be expanded not only to clarify these issues in the technical area, but also so that a user can follow the logic used in the code itself.

Issues such as boundary conditions, time step definition, stability, definition of solution, numerical operators and accuracy, have not been adequately addressed in the report. These issues should be specifically defined.

For FLAG, a line-by-line check of the code is necessary. Discrepancies between the theoretical discussions and what has been programmed have been discovered, one of the most serious being the absence of agglomeration capabilities in the code. A line-by-line check is also necessary to fill in voids in the technical discussion.

In the following section, a recommended outline for future documentation of FLAG is presented. The outline developed is one which will allow a reader to follow the development and operation of the computer model and code in a logical and concise manner. Considerable reqriting of FLAG documentation will be necessary because of a lack of clarity and the omissions in the existing reports.

B. RECOMMENDED OUTLINE FOR COMPUTER CODE DOCUMENTATION

Given below is the recommended outline for documentation of the FLAG computer code. Documentation will be issued in the form of a three volume final report. Volume I will be the technical report describing the physical model, governing equations, and method of solution. Volume II will be the user's manual describing the structure and operation of the computer code. Volume III will be the System Manual.

Volume I will contain the essential fomulations necessary to understand the mathematical relationships which govern the behavior of the models. Unlike the existing FLAG documentation, it will not be a text on hydrodynamic theory. Derivations will not be contained which are better referred to in a text on the subject.

Volume II will be done in careful detail to permit the reader to follow all the way through the codes on a line by line basis. Indeed, it will be possible for the user to make modifications of the code on the basis of the detailed documentation contained in Volume II.

Volume III will be a Systems Manual oriented towards the computer scientists who want to switch the code to a new computer or want to modify the code.

VOLUME I

TECHNICAL VOLUME OUTLINE

(FLAG)

VOLUME II

USER'S MANUAL OUTLINE

(FLAG)

SUMMARY

PREFACE

TABLE OF CONTENTS

I. INTRODUCTION

II. DESCRIPTION OF INPUT/OUTPUT VARIABLES

III. INPUT GUIDE

IV. INPUT/OUTPUT FILES

V. FLOW CHART

VI. DIAGNOSTIC MESSAGES

VII. SAMPLE CASES

1. Input
2. Output
3. Restart

VIII. GENERAL COMMENTS AND OBSERVATIONS

VOLUME III
SYSTEMS MANUAL OUTLINE

II. C. DISCUSSION OF OUTLINE ELEMENTS

1. Summary Tables Relating Major Outline Elements to Existing Documentation and Needed Action

The following tables are a composite detailing the correlation between the available JAYCOR documentation and the proposed FLAG documentation which BDM will develop.

PROPOSED OUTLINE TECHNICAL VOLUME	AVAILABLE DOCUMENTATION	STATUS	REQUIRED ACTION
SUMMARY			NEEDS TO BE WRITTEN
PREFACE			NEEDS TO BE WRITTEN
TABLE OF CONTENTS			NEEDS TO BE WRITTEN
LIST OF ILLUSTRATIONS/TABLES	VOL. I ii VOL. II iii, iv, v	ACCEPTABLE	NONE UNLESS ADDITIONAL TABLES ADDED
NOMENCLATURE	VOL. I APPENDIX A VOL. I SEC 3.6 VOL. I APPENDIX B	INCOMPLETE (SOMETIMES CONFUSING)	NEEDS TO BE UNIFIED
I. INTRODUCTION	VOL. I SEC. 1	INCOMPLETE	NEEDS TO BE REWRITTEN
II. MATHEMATICAL FORMULATION OF MODEL		DOCUMENTATION IMPLIES INCONSISTENCIES IN CODE	NEEDS GENERAL EXAMINATION OF THEORY AND CODING
1. GOVERNING EQUATIONS		INCOMPLETE	THEORY MUST BE EXAMINED AND FORMULATED IN USABLE MANNER
a) FLUIDS	VOL. I SEC. 3 VOL. I SEC. 8	LAMINAR THEORY NOT INCORPORATED	THEORY MUST BE EXAMINED AND CODING VERIFIED
b) PARTICLES	VOL. I SEC. 4 VOL. I SEC. 5 VOL. I SEC. 7 VOL. I SEC. 8	POSSIBLE TROUBLE IMPLIED FROM DOCUMENTATON	THEORY MUST BE EXAMINED AND CODING VERIFIED
2. CHEMISTRY		IMPLIED FROM DOCUMENTATION THAT CHEMISTRY DOES NOT WORK	THEORY MUST BE EXAMINED AND CODING VERIFIED
a) HOMOGENEOUS KINETICS	VOL. I SEC. 5	INCOMPLETE	THEORY MUST BE EXAMINED AND CODING VERIFIED
b) HETEROGENEOUS KINETICS	VOL. I SEC. 5	INCOMPLETE	THEORY MUST BE EXAMINED AND CODING VERIFIED

Figure 1a. Technical Volume - FLAG

PROPOSED OUTLINE TECHNICAL VOLUME	AVAILABLE DOCUMENTATION	STATUS	REQUIRED ACTION
II. MATHEMATICAL FORMULATION OF MODEL (Continued)			
3. CLOSURE EQUATIONS	INCOMPLETE	INCOMPLETE	THEORY AND CODING NEED TO BE EXAMINED
a) LAMINAR MODEL	NONE GIVEN	INCOMPLETE (IN CODE)	MUST BE FORMULATED CODE CHECKED
b) TURBULENT MODEL	VOL. I SEC. 3.3	POSSIBLE INCONSISTENCIES FROM THEORY AND CODE	THEORY AND CODING NEED TO BE EXAMINED
c) DRAG COEFFICIENT MODEL	VOL. I SEC. 4.2	DOCUMENTATION SOMEWHAT VAGUE	MODEL CHECKED, CODING MUST BE CHECKED
4. RADIATION	VOL. I SEC. 8.1 VOL. I SEC. 8.2	ACCEPTABLE	CODING NEEDS TO BE CHECKED
III. GRID	VOL. I SEC. 1	INCOMPLETE	NEEDS TO BE FULLY DEVELOPED
IV. METHOD OF SOLUTION		DOCUMENTATION INCOMPLETE	NEEDS TO BE CONSTRUCTED LINE BY LINE FROM CODE
1. DIFFERENCE FORMULA	VOL. I APPENDIX A	NOT ALL EQUATIONS ARE SHOWN	MUST BE VERIFIED
2 STABILITY AND CONVERGENCE CRITERIA	NONE, EXPLICITLY GIVEN	NONE, EXPLICITLY GIVEN	MUST BE DEVELOPED
3 SOLUTION ALGORITHMS	VOL. I SEC. 3.5	CONFUSING AND INCOMPLETE	MUST BE DEVELOPED
4. GENERALIZED SOLUTION TECHNIQUES	VOL. I SEC. 3.5	CONFUSING AND INCOMPLETE	MUST BE DEVELOPED
REFERENCES	VOL. I SEC. 1.1 VOL. I SEC. 3.7 VOL. I SEC. 4.5 VOL. I SEC. 5.6 VOL. I SEC. 7.8 VOL. I SEC. 8.5	INCOMPLETE	NUMERICAL SOLUTION ALGORITHMS MUST BE REFERENCED, GIVEN REFERENCES MUST BE GROUPED TOGETHER

Figure 1b. Technical Volume - FLAG (Continued)

PROPOSED OUTLINE USER'S MANUAL	AVAILABLE DOCUMENTATION	STATUS	REQUIRED ACTION
SUMMARY			NEEDS TO BE WRITTEN
PREFACE			NEEDS TO BE WRITTEN
TABLE OF CONTENTS			NEEDS TO BE WRITTEN
I. INTRODUCTION	VOL. II SEC. 1	INCOMPLETE	NEEDS TO BE REWRITTEN
II. DESCRIPTION OF INPUT/ OUTPUT VARIABLES	VOL. II SEC. 3.1 VOL. II SEC. 4	INCOMPLETE	NEEDS TO BE DEVELOPED
III. INPUT GUIDE	VOL. II SEC. 3.1	INCOMPLETE	NEEDS TO BE REWRITTEN
IV. INPUT/OUTPUT FILES	NOT EXPLICITLY STATED (SOME HELP VOL. II SEC. 4)	CLEAR DESCRIPTION AND USE OF FILES DOES NOT EXIST	NEEDS TO BE REWRITTEN
V. FLOW CHART	VOL. II SEC. 4	TOO CUMBERSOME, LACKS CLARITY	NEEDS TO BE DEVELOPED
VI. DIAGNOSTIC MESSAGES	VOL. II SEC. 3.6	ONLY A FEW SPECIFIC EXAMPLES MENTIONED	NEEDS TO BE DEVELOPED
VII. SAMPLE CASE	VOL. II SEC. 7 VOL. II SEC. 6	NO UNIFIED CASE	NEEDS TO BE DEVELOPED
1. INPUT	VOL. II SEC. 3.1 VOL. II SEC. 3.2	UNCLEAR	NEEDS TO BE ORGANIZED
2. OUTPUT	VOL. II SEC. 3.8	UNCLEAR	NEEDS TO BE ORGANIZED
3. RESTART	VOL. II SEC. 3.9 VOL. II SEC. 2.6	UNCLEAR	NEEDS TO BE MADE CLEAR
VIII. GENERAL COMMENTS AND OBSERVATIONS	NONE	DOES NOT EXIST	NEEDS TO BE DEVELOPED

Figure 2. User's Manual - FLAG

2. Detailed Description Of Major Outline Elements Of FLAG

The discussion presented will focus on the major proposed outline elements. First the purpose and content of each element's final documentation will be discussed. Second, the status of the existing documentation and code section relating to the final outline element is given. Finally, the actions we will take to complete the documentation are detailed.

The numbering is consistent with the numbering in section B. Section C-1 can be used as a handy guide to major conclusions.

TECHNICAL VOLUME - FLAG

SUMMARY

Purpose of Section

This section presents a synopsis of the JAYCOR FLAG computer model including comments on the computer code's applicability for analyzing coal gasifiers.

Status

Does not exist in available documentation.

Action Required

Section needs to be written.

PREFACE

Purpose of Section

This section acknowledges the contracting agency and contract number as well as any contributions made to this program by individuals not specifically listed as authors.

Status

Does not exist in the available documentation.

Action Required

Section needs to be written.

<u>TABLE OF CONTENTS</u>

This section is self-explanatory.

<u>LIST OF ILLUSTRATIONS AND TABLES</u>

This section is self-explanatory.

<u>NOMENCLATURE</u>

This section is self-explanatory.

(SECTION I) INTRODUCTION

Purpose of Section

In this section, the FLAG computer model will be presented. The section will discuss the physics of coal gasifiers and the assumptions made in arriving at the final FLAG model. In addition to discussing the physics of the problem, the numerical techniques used in solving the equations will be discussed. This section will include all of the justifications and assumptions made in the physical model and solution techniques.

Status

The available documentation does not present a clear and concise discussion of FLAG. In addition, extraneous information is presented which is not relevent to FLAG (e.g., the structural deformation of caking coal particles in pyrolysis).

Action Required

This section needs to be written and structured consistent with the final FLAG model to be delivered to DOE/METC.

(SECTION II) MATHEMATICAL FORMULATION OF MODEL

(SECTION II 1) Governing Equations
(SECTION II 1a) Fluids

Purpose of Section

In this section, the equations describing the fluid motion will be presented. This will encompass the conservation laws for mass, momentum and energy. The equations will be given in differential form with appropriate references so that, if the reader desires, he can follow the development of the differential equations from first principles. Also to be discussed in this section are the initial and boundary conditions.

Status

The governing fluid equations are discussed or presented in a number of sections in the available documentation. However, the equations are not presented in a fully conserved form. In particular, energy is not solved for in a conserved form. The consequences of this are the possibilities of creating instabilities in the flow field. This will lead to incorrect solutions and will not permit FLAG to be used as a predictive tool. In addition, the equations as presented are incorrect for modeling of flows with low or high Reynold's numbers. In the documentation, laminar viscosity is completely ignored. Hence, the system of equations is incapable of modeling low Reynolds number flow. Bulk viscosity and terms related to flow compressibility have been ignored. Therefore, flows with high Reynolds numbers cannot be properly treated. The initial and boundary conditions are not presented in the available documentation. These conditions are a necessary and required part of any formulation of fluid equations.

Consequently, the presented FLAG flow system does not realistically model coal gasification. This eliminates FLAG's ability to be used as a computational tool in aiding in the design of coal gasifer systems.

Action Required

The system of equations will be recast in a fully conservative form, in order to eliminate instability issues which usually arise in attempting to solve fluid equations posed in their primitive variable form. The relevant terms ignored in the FLAG system of equations will be restored. Inconsistencies observed between the posed and coded equations, (e.g., incorporation of laminar viscosity), will be eliminated via a reconstruction of the implemented model. In addition, the initial and boundary conditions which are not specified in the available documentation will be obtained from a line by line reconstruction of the computer code.

(SECTION II) MATHEMATICAL FORMULATION OF MODEL

(SECTION II 1) Governing Equations

(SECTION II 1b) Particles

Purpose of Section

The governing equations for particles will be discussed in this section. The equations of motion and energy conservation will be presented in differential form. Also to be discussed are the drag forces and energy contributions to the fluid flow field due to the presence of particles. The initial and boundary conditions will be presented.

Status

The formulation of the particle motion and energy is generally well posed in the availiable documentation. The only issue of note in clarification is the relationship between the drag force and the drag slowing down frequency used in the particle motion equation. As in the case of the the fluid equations, initial and boundary conditions are not stated.

Action Required

The initial and boundary conditions will be reconstructed by a line by line examination of FLAG.

(SECTION II) MATHEMATICAL FORMULATION OF MODEL

(SECTION II 2) Chemistry

(SECTION II 2a) Homogeneous Kinetics

Purpose of Section

This section presents the homogeneous chemistry processes occurring in coal gasifier systems. In addition to the chemistry processes described in the available documentation, additional chemistry processes will be incorporated to allow for a flexibility in the model which presently does not exist.

Status

The FLAG homogeneous chemistry model does not treat any kinetics processes. The assumed reactions are either instantaneous or in equilibrium. This model is very restrictive and allows the user no flexibility. In addition, CH_4 kinetics is ignored in the present model because it is assumed to be slow. This assumption is too restrictive and CH_4 kinetics should be incorporated, thus allowing the model to dictate the magnitude and importance of CH_4 kinetics. Even beyond this, the user should have total flexibility in selecting and inputting any arbitrary kinetic package and associated rate coefficients. This will allow the user to address the complex chemical reaction issues necessary for the modeling of coal gasifiers.

Action Required

In addition to the homogeneous chemistry mechanism presented in the available documentation, an option will be included in the computer code to allow the user to input any general reaction mechanism of the form $A + B + C \rightarrow D + E + F$ with their associate rate coefficients given in the Arrhenius form (i.e., $k = AT^{-N}e^{-B/RT}$).

(SECTION II) MATHEMATICAL FORMULATION OF MODEL
(SECTION II 2) Chemistry
(SECTION II 2b) Heterogeneous Kinetics

Purpose of Section

The purpose of this section os to discuss the model of the heterogeneous kinetics and devolatilization process incorporated in the FLAG computer model. This will include a time-dependent devolatilization model.

Status

The present FLAG model assumes devolatilization occurs instantaneously. It is naive to make such a simplistic assumption of devolatilization in coal gasifiers. Such a model induces bubbles and incorrect heterogeneous kinetics effects that are not consistent with the actual development of the coal gasifier field. Devolatilization is dependent upon particle sizes, temperatures, etc. Instantaneous devolatilization ignores the fact that the numerical solution proceeds over variable integration time steps which are developed based upon the physics and numerical solution operators. The existing model is too elementary to be used in analyzing the complex physics of coal gasifiers.

The char/oxygen reaction stated restricts itself to low-temperature operations. The reaction should be extended to yield both CO and CO_2 to eliminate the imposed operational limitation inherent in the reaction as stated.

Action Required

A time-dependent devolatilization model will be developed consistent with the work of A.F. Sarofim and J.W. Beer (DOE/WVU Conference on Fluidized Bed Combustion, Oct. 27-29, 1980). This model will be coded into the computer code and sensitivity runs will be performed to show the influence to time-dependent devolatilization on the reactor flow field.

The char/oxygen reaction will be extended to yield as products both CO and CO_2. The references for the rate constants for this reaction, in addition to the char-water and carbon dioxide reactions (which are not given in the available documentation) will be included.

(SECTION II) MATHEMATICAL FORMULATION OF MODEL

(SECTION II 3) Closure Equations
(SECTION II 3a) Laminar Model

Purpose of Section

The model which treats laminar mixing will be discussed in this section.

Status

Laminar mixing is ignored in the available documentation of the fluid equations. However, laminar mixing is addressed in the computer code and uses Sutherland's law which is strictly valid only for air. No documentation is provided for the justification of using Sutherland's law.

In the Introduction of the Technical Volume, reference is made to the IGT cold-flow experiment. Strong concerns exist in the applicability of the present code as documented to the modeling of this experiment because of inconsistencies between documentation and implementation of laminar terms which are relevant to this experiment. The attainment of the objective of providing a practical engineering tool is, therefore, questionable.

These concerns are magnified as the result of exercising FLAG in the laminar regime (i.e., where turbulent effects are negligible). Computer results showed highly diffusive effects totally inconsistent with laminar theory. Even when additional computer calculations were performed where all modeled diffusive effects were specifically set equal to zero, the computer calculations still showed large diffusional effects, indicating that the present code cannot model the laminar regime.

The numerical scheme used to solve the fluid equations is highly suspect since it appears that the numerical scheme is inducing large artificial diffusional effects into the problem. Consequently, any attempt to compare computer results with experimental data (e.g., bubble formation, jet penetration as shown in Figures 6-3 through 6-5, gas flow patterns, temperature fields) is inappropriate until this major problem is dealt with and corrected.

Action Required

A comprehensive examination of all diffusive quantities and their numerical effects will be undertaken. The interrelationships between these effects must be addressed in order to correct the major problem areas of FLAG.

(SECTION II) MATHEMATICAL FORMULATION OF MODEL

(SECTION II 3) Closure Equation
(SECTION II 3b) Turbulent Model

Purpose of Section

In this section the turbulence model will be discussed.

Status

At present, there are no major reservations regarding the specific turbulence model proposed; however, the applicability of this turbulence model can only be established via comparisons between computer calculations and experimental data. However, implementation of this model in the code is suspect because of results described below.

FLAG has been exercised for the effects of mixing in a configuration of concentric jets in a pipe. For these computer runs, the turbulent mixing length, l_m, was varied over a range of two orders of magnitude. The results showed no variation with turbulent mixing length, i.e. the results were identical. This result is totally inconsistent with the proposed turbulence model which should scale with l_m.

Examination of the turbulent viscosity subroutine shows that the viscosity is a function of three terms. These terms are the turbulent coefficient, the laminar coefficient and a convective coefficient which is interpreted as a turbulent transport property. An order of magnitude check of each of these three coefficients showed that the convective coefficient is overwhelmingly the largest. Thus, the computer code uses this coefficient to compute mixing rates, i.e. diffusion. While use of a convective diffusion coefficient is conceptually acceptable, the incorporation of such a coefficient must be carefully implemented. Problems arise in FLAG due to incorrectly implementing such an artificial term. When implementing such a method, two issues must be addressed. First, the term is used only to maintain numerical stability. This approach is a consequence of the failure to correctly incorporate higher order terms in the governing differenced fluid equations, which usually is done by most successful time dependent fluid codes (APACHE, RICE, RAVEN). Second, the convective term must only stabilize the numerical solution and not affect the structure of the flow field, which is physically controlled by the laminar and turbulent mixing rates. In FLAG in the turbulent subroutine these terms are not properly implemented.

However, there are more significant problems in FLAG relating to diffusive properties. These properties are numerical in nature indicating errors in the numerical scheme or its implementation in FLAG. Computer runs with all physical diffusion coefficients set equal to zero produced results showing extremely rapid mixing effects, i.e., large diffusive effects. This is inconsistent with laminar/turbulent theory. This indicates a major flaw on the FLAG computer code.

This major flaw eliminates all possibilities of performing any meaningful comparisons between calculated results and experimental data (see section IV). Thus, the generated data calculated by FLAG is not consistent with the stated theoretical model.

Action Required

A comprehensive examination of all diffusive quantities and their numerical effects will be undertaken. The interrelationships between these effects must be addressed in order to correct the major problem areas of FLAG.

(SECTION II 3) Closure Equations

(SECTION II 3c) Drag Coefficient Model

1) Purpose of Section

This section will present the drag coefficient model including experimental data for particles in coal gasifiers including all necessary references for the experimental data.

2) Status

The drag coefficient model is well posed in the available documentation. Charts are also presented which give the drag coefficient as a function of void fractions and Reynold's number. These charts will be incorporated in the proposed documentation.

3) Action Required

The present section is adequate and will be included with minor rewriting.

(SECTION II 4) Radiation

1) Purpose of Section

This section will discuss the radiation transfer equations incorporated in the FLAG computer model.

2) Status

The radiation model is presented in considerable detail in the available documentation.

3) Action Required

In the proposed documentation only the final equations specifically evaluated in the computer code will be discussed. References will be given to allow the reader to address the fundamental development of the final equations.

(SECTION III) NUMERICAL GRID

PURPOSE OF SECTION

In this section, the numerical grid upon which the numerical difference equations are based will be discussed. Issues such as boundary relationships between the physical reactor vessel and its numerical grid approximation will be presented. This section will also describe how reactor boundaries are specified as input to the computer code.

STATUS

The rectangular numerical zone structure, i.e. the grid, implemented in the FLAG computer code is a basically acceptable methodology. However, extreme care must be taken when this grid is used to approximate nonrectangular surfaces. This area of concern will impact cases involving flow in expanding channels, specifically the nozzle-like sections of a gasifier. In particular, the creation of nonphysical recirculation zones must be addressed, as well as artificially induced turbulent behavior in the flow fields. These topics are not dealt with in the documentation of FLAG and considerable ambiguity is shown in the related boundary conditions as specifically implemented on the given grid system. Note the graphics, given in the documentation figure 5-1, in which particles are shown to reside in areas outside the reactor vessel's proposed surfaces and yet are still in the flow field. This grid formulation can severely limit FLAG'S predictive capabilities unless extreme case is taken when formulating the boundary conditions.

ACTION REQUIRED

The inherent problems of rectangular grids modeling nonrectangular surfaces must be addressed through the running/exercising of the FLAG computer code on simple cases, in order to determine the magnitude of this problem. Also, a reconstruction of the computer code's boundary condition/grid interrelationships must be accomplished via an examination of the actual coding.

This entire section needs to be written since it is not discussed in the available documentation.

(SECTION IV) METHOD OF SOLUTION

(SECTION IV 1) Difference Formula

Purpose of Section

This section will show how the governing equations which are presented in their differential form in Section II are recast into their difference form.

The generalized form of first and second order operators will also be presented to aid the reader in understanding the evolution to the differenced form from the differential form. The form of the difference equations along the reactor boundaries will also be presented.

Status

The differenced form of the equations is presented (except along the reactor boundaries) in the available documentation. However, there are a few typographical errors (e.g.-failure to show bars over all quantities consistent with the differencing scheme). It would be helpful to the user if the generalized differenced form of the first and second order operators were presented prior to stating the fully developed differenced form. This would assist the comprehension of exactly how the differenced forms evolve from the model's differential equations. These operators are not given in the available documentation.

Required Action

It will be necessary to correct the typographical errors in the presented differenced equations. In addition, the generalized first and second order operators will be formulated and presented. The differenced equations along the reactor boundaries will be reconstructed from a line-by-line examination of the computer code.

(SECTION IV) METHOD OF SOLUTION

(SECTION IV 2) Stability and Convergence Criteria

Purpose of Section

The purpose of this section is to: (i) present the stability criteria for the fluid and particle physics and (ii) the convergence criteria for the solution algorithms.

Status

There are no stability criteria explicitly incorporated in the computer code. Also, none is input as data into the computer code in data statements, common blocks, etc. The user is expected to input time steps limits, (i.e., minimum and maximum time steps); however, the user is given no information regarding the establishment of these limits. This assumes the user is well versed in time dependent computational fluid dynamic analysis.

There is a specific value for the iterative convergence criteria built into the computer code. Whether this criteria is valid for various sets of operating conditions can only be verified by exercising FLAG over a wide range of conditons. Note that the establishment of a convergence criteria is highly dependent upon the accuracy desired in the final solution and the integration time step.

Required Action

Stability criteria will be developed which the computer code will use to automatically select the time step required for integration. These stability criteria will account for convective effects, diffusional effects, chemistry, etc., (i.e., all terms not solved implicitly in the numerical analog).

The computer code will be exercised over a wide range of operating conditions and integration time steps to define acceptable values for the convergence criteria. The results of this will be incorporated in this section to enhance the user's ability to run FLAG.

(SECTION IV) METHOD OF SOLUTION

(SECTION IV 3) Solution Algorithms

Purpose of Section

This section will focus on how the equations discussed in Section IV-1 are solved. It will deal with the mathematical techniques required to numerically solve the differenced equations governing fluid-particle motion, energy, mass, chemistry, etc. In particular, this section will discuss the Newton-Raphson iterative methodology coupled to the implicit solution techniques of FLAG (i.e., Crank-Nicholson, Kansa and ICE).

Status

The coupling of the Newton-Raphson technique with the implicit algorithms in FLAG should in theory produce accurate and rapidly converging solutions. Unfortunately, this is not the case in FLAG. Exercising the code shows that for large time steps (on the order of the fluid-convective time across a computational cell) the solution methodology is not nearly as efficient as would be expected from implicit schemes. Calculations made using these large time steps required 21 iterations to converge. This is inconsistent with the documentation which states that only 3 to 4 iterations are required when operating in this time step regime. This points to an improper implementation of the stated numerical techniques in FLAG. Additional calculations for which the time step was reduced to the acoustical limit (consistent with the CFL limit) required 3 to 4 iterations for convergence. This also points to an improper implementation of the numerical scheme. If indeed this methodology is limited to many iterations even at the acoustical limit, then explicit operators should be seriously considered. The reasons for this are: (i) ease of coding, (ii) iterations not required and (iii) computationally faster.

Action Required

The numerical scheme incorporated in FLAG will be reconstructured to determine if the technique has been improperly implemented in the computer code. If it is found that the technique has been improperly implemented then the necessary corrections will be made. If the method is correctly implemented, considerations will be given to other solution techniques.

(SECTION IV) METHOD OF SOLUTION

(SECTION IV 4) Generalized Solution Technique

Purpose of Section

In this section, the overall solution technique will be discussed. The section will focus on how all of the equations which have been stated to define the fluid-particle processes, occuring in coal gasifiers, are sequentially evaluated to arrive at a solution. This section will be analogous to a top-level flowchart. It will allow the reader to understand the logic used in the computer code in solving the equations.

Status

Some of this information is available in the documentation, but it is incomplete and confusing. The available information is not nearly as detailed as required.

Required Action

This section needs to be developed consistent with the final form of FLAG.

USER'S MANUAL - FLAG

(Section I) Introduction

a) Purpose and Content

This section will present a description of the User's Manual's structure.

b) Status of Documentation

The new introduction must track the new documentation and therefore is presently incomplete.

c) Actions to be Taken

This section needs to be rewritten.

(Section II) Description of Input/Output Variables

a) Purpose and Content

All relevant variables necessary to run the computer code will be explained. Also, incorporated and discussed in this section will be the output variables generated during the execution of the code. This section will contain enough clarity so that the reader will not have to refer to the Technical Volume to comprehend the variable's function.

b) Status of Documentation

The existing documentation presented in Volume II, sections 3.1 and 4 is not complete. As easily comprehended section relating to all output variables is missing.

c) Action to be Taken

This section must be developed. For example, the code will contain a representative set of kinetic parameters. A default option will allow the user to input different reactivity constants or values for the ratio of CO and CO_2 produced in the char-oxygen reactions. Constants for a number of different coals, are included in our task 3.1 topical report.

(Section III) Input Guide

a) Purpose and Content

This section will present all necessary information needed to run the computer code. Also, various options available to the user will be explicitly discussed.

Examples of the kind of information which will be included are: (1) modification of the mesh structure, (2) options on printing output data, (3) use of graphics (if incorporated) and, (4) discussion of restart capabilities.

b) Status of Documentation

The present documentation is incomplete. For example, no comprehensive instructions for restart capabilities are given.

c) Actions to be Taken

This needs to be rewritten.

(Section IV) Input/Output Files

a) Purpose and Content

This section will discuss the nature of the input and output files, i.e., formating, names, memory sizes.

b) Status of Documentation

No explicit description of Input/Output files is given.

c) Actions to be Taken

This section needs to be developed. The subsequent discussion will be based on experience and the final form of the FLAG computer code.

(Section V) Flow chart

a) Purpose and Content

This section will present a detailed flow chart of the computer code.

The structure of the computer code will also be discussed in this section with additional comment statements incorporated in the computer code to allow the user to easily identify the calculations being performed with the numerical model discussed in the technical report.

b) Status of Documentation

Considerable detail relating to flow charts is available in the existing documentation. However, the material is cumbersome and is not clear.

c) Actions to be Taken

A flow chart which represent the final configuration of the code must be developed.

(Section VI) Diagnostic Messages

a) Purpose and Content

This section will discuss diagnostic comments, error messages, etc., to be incorporated in the computer code which aid the user.

Checks of inconsistencies in input conditions, time step requirements, development of instabilities, etc., will be incorporated in the computer code, as well as messages printed to inform the user of potential problems.

b) Status of Documentation

Diagnostic messages are not explicitly stated in the documentation.

c) Actions to be Taken

These messages will be added where appropriate as the program progresses.

(Section VII) Sample Cases

a) Purpose and Content

In this section, sample cases will be presented to allow a new user to verify that the computer code is running properly. The case being exercised will first be discussed. Also, a listing of the input will be shown and with its generated output. By presenting sample cases in this manner, the user can independently establish his own input file and then compare it with the sample input file to verify that he is correctly following the input guide in Section III. Also, the user can compare the results with the sample output. Cases will be presented for both cold and restart cases.

The sample cases will show all of the required job control language information.

b) Status of Documentation

No case is present in the documentation which shows the user the complete sequence of running this code, including using the restart capabilities.

c) Actions Required

The actual sample cases incorporated will be cases run during the performance of Tasks 3.3 - 3.7.

Only that information which is necessary to convince a new user that he has exercised FLAG successfully will be included.

(Section VIII) General Comments and Observations

a) Purpose and Content

Within this section general comments and observations will be made regarding the execution and application of the computer code. During the performance of tasks in this program information will be obtained which will be beneficial to other users. This section is structured in order to make this information available to them. It will include helpful comments on observed limitations, suggested input variables, etc. This information is not available in the present documentation.

b) Status of Documentation

No such section exists in the present documentation.

c) Actions to be Taken

This section will be developed.

SYSTEMS MANUAL
OUTLINE

VOLUME III
SYSTEMS MANUAL

The purpose of the systems Manual Volume is to provide detailed material and descriptions relating to the structure and operation of the computer code. It is prepared for computer scientists, systems level analysts, and programmers whose responsibilities are major modifications to the computer code, transfering the computer code to other operating systems, resolution of program/system problems, etc. This volume is not being written for the physicists or engineering users of the computer code. The Technical and User's Volumes will be prepared for these individuals.

PREFACE

This section will discuss the purpose of this volume. Reference will be made to the Contracting Agency and Contract Number.

I. INTRODUCTION

The purpose of this section is to discuss the structure of this volume.

II. FUNDAMENTALS

This section will discuss the overall philosophy of the structure of the code. This will include hardware considerations, handling of input/output files, restart considerations and diagnostic messages which are system specific. This section will serve as a general background for the remainder of this volume.

III. DATA BLOCKS

This section will present the data blocks incorporated in the code (i.e., common blocks, equivalenced data, initilization data, parameter statements, etc.) as well as an explanation of the variables. The Fortran variables will be listed along with information on their type, dimensions, and a cross reference for the subroutines and common blocks which contain them.

IV. MODULES

This section will discuss the modules which comprise the code. The function of each of the modules will also be discussed.

V. SUBROUTINES

This section will address the subroutines which comprise each of the modules. The utility subroutines will also be addressed in this section .

VI OPERATIONAL SYSTEM INTERFACES

This section will discuss the job control language necessary for executing the computer code.

VII CODE MODIFICATIONS/ADDITIONS

This section will discuss how the computer code can be modified and how these changes are implemented.

D. RECOMMENDED PLAN TO COMPLETE DOCUMENTATION

1) Discussion

a) Reconstruction of Documentation

The confusing documentation relating to the numerical techniques is unacceptable and must be addressed before the exercise tasks can be properly carried out. The situation is considerably complicated by the fact that fundamental errors in the coded numerical technique are present. This is born out by the fact than FLAG cannot model flow in a pipe. Other errors exist in FLAG; however, they are minor in comparison to the numerical issue.

As shown in figure 3, the reconstruction activity will be scheduled over the next 4 month period. This reconstruction activity may identify code modifications that are necessary and which would be performed under Task 3.6, Modification of Models/Codes. The reconstruction of the documentation will result in a baseline for further improvements and modifications.

b) Final Documentations

The documentation will be presented in three volumes. Volume I will cover technical issues, Volume II will be a user's manual and Volume III wil be a systems manual. The outline of each volume is presented in section B. In addition, an extensive appendix of relevant reference material will be either included with the Technical Volume or presented separately.

c) Documentation Input

The reconstruction described above will provide the base revised documentation material. As the program proceeds, input material will be generated in the code exercise tasks (3.3, 3.4, 3.5). Experience with system files, necessary default options, etc., are some of the types of documentation input we will gain from these tasks. Modifications approved under Task 3.6 will form a second source of revisions for both the documentation and the code itself.

2) Schedule

The necessary reconstruction of the documentation is scheduled for a 4 month period, as shown in figure 3. To avoid a severe impact on the scheduled exercising of the code in Task 3.3, we will stage the documentation reconstruction activity. First, we will reconstruct the gas-fluid algorithms. This can then be used in exercising some of standard flow conditions in Task 3.3a appropriate for FLAG. The particle-fluid algorithms will be treated next, followed by the chemistry algorithms. The dotted line labeled 1 in figure 6 denotes this interaction between reconstruction and exercising activity. The line labeled 2, denotes modifications that may be necessary because of information developed during the reconstruction.

Changes in the code or documentation that are found to be necessary during performance of Task 3.3, as well as Tasks 3.4, 3.5, and 3.7, will be made under Task 3.6 and included in the documentation as illustrated by the dotted line 4 in figure 6. Other changes that are found to be necessary will be made in Task 3.6 and included in the documentation.

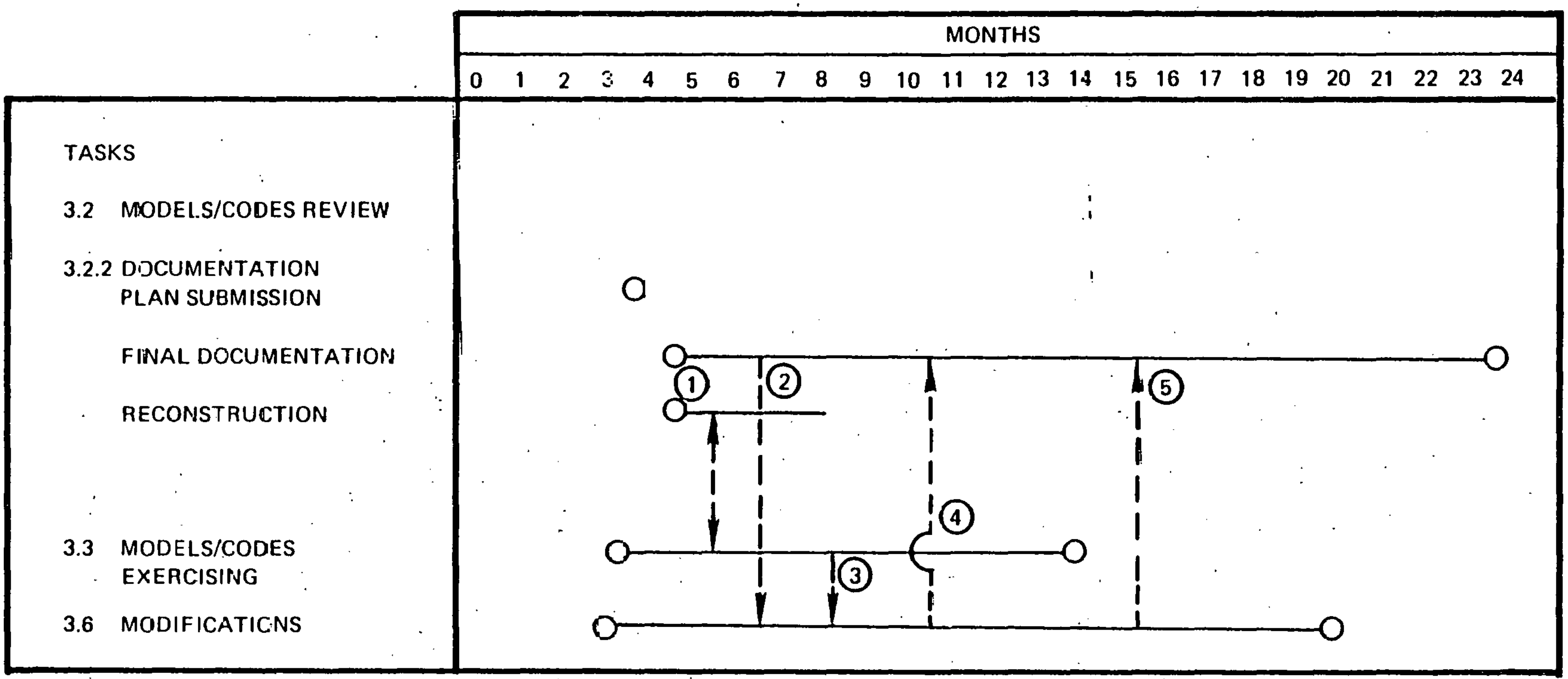
3) Communication and Logging of Modifications

a) Regarding Documentation

The present plan devotes a separate page and discussion to each major section of the final documentation. This format will be converted into a loose leaf set of volumes. As sections of the documentation are reconstructed they will be inserted in the loose leaf folders. The same volumes can be updated as additional sections are rewritten or updated. A separate volume will collect material that is replaced. Separate sets of volumes will be kept at METC, BDM and Exxon. The monthly technical progress report will be the vehicle for transmitting sections of the documentation.

b) Code Modifications and Transmission of Modifications

Two separate copies of each code (CHEMFLUB and FLAG) will reside on the BDM-VAX computer system in Washington, D.C. One copy will only be accessed by one user responsible for both updating and



(1) RECONSTRUCTION PROCEEDS WITH CONCURRENT EXERCISING

(2) MODIFICATIONS OF THE CODE MAY BE NECESSARY AND WILL BE DONE UNDER TASK 3.6

(3) MODIFICATIONS NEEDED AND IDENTIFIED DURING EXERCISING WILL BE DONE UNDER TASKS 3.6

(4) MODIFICATIONS WILL BE INCLUDED IN DOCUMENTATION UPON APPROVAL BY DOE

(5) FURTHER MODIFICATIONS WILL BE REQUIRED AS A RESULT OF TASKS 3.4 AND 3.5

Figure 3. Schedule - FLAG

documenting changes to this copy. The record of the alterations and modifications will be done via comment statements in the code and a written log stating the changes. The other copy will be a working copy of the updated code accessed by all users. As problems are successfully addressed the required modifications will be given to the one user responsible for the one copy which is used only for documentation. Only this person will update the documented version. This allows for a simple path of information flow.

On a monthly basis, the changes for each code will be transmitted to METC along with a copy of the associated written log. This procedure after the next 4 months (completion of reconstruction) will be done on a quarterly basis.

c) Technical Communication

It is strongly recommended that METC interact with BDM on two levels. First, METC technical staff should come to Albuquerque and spend a period of time consistent with their learning about our technical plans and the resulting required actions. Second, METC should link to the BDM-VAX in Washington, D.C. to facilitate the monthly transfer of the changes.

CHAPTER III
CHEMFLUB

A. GENERAL COMMENTS

The discussion of the technical details of System, Science and Software's CHEMFLUB computer model is most lacking in the treatment of the numerical formulation. The technical report does not discuss or demonstrate which differencing schemes are used and how they are solved. However, the discussion on the differential equations is acceptable.

The main difficulty with the CHEMFLUB technical volume is that it is not written as a technical volume to a computer model. All of the technical details that allow translation from the theory to a working computer model are missing (e.g., boundary conditions, stability, solution techniques, etc.). This information will have to be obtained from a check of the code itself.

Within the user's manual, the prime area of concern is the input guide. This section will have to be rewritten. It is in a form which is confusing to a user. The user guide should be user oriented and helpful to the user with operational insight given based on the author's experiences with the computer code.

B. RECOMMENDED OUTLINE FOR COMPUTER CODE DOCUMENTATION

Given below is the recommended outline for documentation of the System, Science and Software CHEMFLUB computer code. Documentation will be developed in the form of a three volume final report. Volume I will be the technical report describing the physical model, governing equations, and method of solution. Volume II will be the user's manual describing the structure and operation of the computer code. Volume III will be a systems manual.

VOLUME I
TECHNICAL VOLUME OUTLINE
(CHEMFLUB)

VOLUME II
USER'S MANUAL OUTLINE
(CHEMFLUB)

VOLUME III
SYSTEMS MANUAL OUTLINE

C. DISCUSSION OF OUTLINE ELEMENTS

1. Summary Tables Relating Major Outline Elements to Existing Documentation and Needed Action

The following tables are a composite detailing the correlation between the existing System, Science, and Software documentation and the proposed CHEMFLUB documentation which BDM will develop.

PROPOSED OUTLINE TECHNICAL VOLUME	AVAILABLE DOCUMENTATION	STATUS	REQUIRED ACTION
SUMMARY			NEEDS TO BE WRITTEN
PREFACE			NEEDS TO BE WRITTEN
TABLE OF CONTENTS			NEEDS TO BE WRITTEN
LIST OF ILLUSTRATIONS/TABLES			NEEDS TO BE WRITTEN
NOMENCLATURE	VOL. II SEC III.3.1 VOL. III SEC. II.2.1	INCOMPLETE	NEEDS TO BE GROUPED TOGETHER AND EXPANDED UPON
I. INTRODUCTION	VOL. II SEC. II VOL. III SEC. I	INCOMPLETE AND NEEDS TO RELATE ONLY TO CHEMFLUB	NEEDS TO BE REWRITTEN
II. MATHEMATICAL FORMULATION OF MODEL		INCOMPLETE	SECTION MUST BE WRITTEN WITH COMPLETE DOCUMENTATION
1. GOVERNING EQUATIONS		NOT GIVEN IN CLEAR FASHION	SECTION MUST BE PRESENTED IN CLEARER MANNER
a) FLUIDS	VOL. II SEC. III.3.1 VOL. III SEC. II.2.2	ACCEPTABLE — BUT NOT SHOWN IN FORM WHICH IS SOLVED BY CODE	NEEDS TO BE CHECKED AGAINST CODE
b) PARTICLES	SAME AS ABOVE	SAME AS ABOVE	SAME AS ABOVE
2. CHEMISTRY		NEEDS DOCUMENTATION; MODELS UNVERIFIED	MODEL MUST BE VERIFIED AND CODING CHECKED
a) HOMOGENEOUS KINETICS	VOL. II SEC. III.3.1 VOL. III. SEC. II.2.3	INCOMPLETE, SOME RATE CONSTANTS NOT DOCUMENTED	MODEL MUST BE VERIFIED AND CODING CHECKED
b) HETEROGENEOUS KINETICS	VOL. II SEC. III.3.1 VOL. III SEC. II.2.3	INCOMPLETE, SOME RATE CONSTANTS NOT NOT DOCUMENTED	MODEL MUST BE VERIFIED AND CODING CHECKED

Figure 4a. Technical Volume - CHEMFLUB

PROPOSED OUTLINE TECHNICAL VOLUME	AVAILABLE DOCUMENTATION	STATUS	REQUIRED ACTION
II. MATHEMATICAL FORMULATION OF MODEL (Continued)			
3. CLOSURE EQUATIONS		NEEDS DOCUMENTATION; MODELS UNVERIFIED	MODEL NEEDS TO BE VERIFIED AND CODING CHECKED
a) LAMINAR MODEL	VOL. II SEC. III.3.1	EMPIRICALLY DERIVED, DATA NOT EXPLICITLY GIVEN	MODEL MUST BE VERIFIED AND CODING CHECKED
b) TURBULENT MODEL	VOL. II SEC. III.3.1	EMPIRICALLY DERIVED, DATA NOT EXPLICITLY GIVEN	MODEL MUST BE VERIFIED AND CODING CHECKED
c) DRAG COEFFICIENT MODEL	VOL. II SEC. III.3.1	EMPIRICALLY DERIVED, DATA NOT EXPLICITLY GIVEN	MODEL MUST BE VERIFIED AND CODING CHECKED
4. RADIATION	VOL. II SEC. III.3.1	ACCEPTABLE	MUST CHECK TO SEE IF IT IS IN CODE CORRECTLY
III. GRID	VOL. II SEC. 3-2	INCOMPLETE	MUST BE DELIVERED
IV. METHOD OF SOLUTION		DOCUMENTATION INCOMPLETE	NEEDS TO CONSTRUCTED LINE BY LINE FROM CODE
1. DIFFERENCE FORMULA	NONE	NONE	MUST BE DEVELOPED
2. STABILITY AND CONVERGENCE CRITERIA	NONE	NONE	MUST BE DEVELOPED
3. SOLUTION ALGORITHMS	VOL. II SEC. III.3.2	INCOMPLETE	MUST BE DEVELOPED
4. GENERALIZED SOLUTION TECHNIQUES	VOL. II SEC. III.3.2	INCOMPLETE	MUST BE DEVELOPED
REFERENCES	VOL. I REF VOL. II REF	INCOMPLETE	BASIC REFERENCES FOR NUMERICAL SOLUTION NEEDED AND GIVEN REFERENCES MUST BE GROUPED TOGETHER

Figure 4b. Technical Volume - CHEMFLUB (Continued)

PROPOSED OUTLINE USER'S MANUAL	AVAILABLE DOCUMENTATION	STATUS	REQUIRED ACTION
SUMMARY			NEEDS TO BE WRITTEN
PREFACE			NEEDS TO BE WRITTEN
TABLE OF CONTENTS			NEEDS TO BE WRITTEN
I. INTRODUCTION	VOL. III SEC. I	INCOMPLETE	NEEDS TO BE REWRITTEN
II. DESCRIPTION OF INPUT/OUTPUT VARIABLES	VOL. III SEC. 3.4 VOL. III SEC. 5	UNCLEAR	NEEDS TO BE REWRITTEN
III. INPUT GUIDE	VOL. III SEC. 5	UNCLEAR	NEEDS TO BE REWRITTEN
IV. INPUT/OUTPUT FILES	NOT EXPLICITLY STATED	CLEAR DESCRIPTION AND USE OF FILES DOES NOT EXIST	NEEDS TO BE REWRITTEN
V. FLOW CHART	VOL. III SEC. 3	INCOMPLETE	NEEDS TO BE DEVELOPED
VI. DIAGNOSTIC MESSAGES	NOT EXPLICITLY STATED	DOES NOT EXIST	NEEDS TO BE DEVELOPED
VII. SAMPLE CASE	VOL. III APPENDIX A	CASE GIVEN	NEEDS TO BE DEVELOPED
1. INPUT	VOL. III APPENDIX A	UNCLEAR	NEEDS TO BE REWRITTEN
2. OUTPUT	VOL. III APPENDIX A	UNCLEAR	NEEDS TO BE ORGANIZED
3. RESTART	VOL. III APPENDIX A	UNCLEAR	NEEDS TO BE MADE CLEAR
VIII. GENERAL COMMENTS AND OBSERVATIONS	NONE	DOES NOT EXIST	NEEDS TO BE DEVELOPED

Figure 5. User's Manual - CHEMFLUB

2. Detailed Description of Major Outline Elements of CHEMFLUB

The discussion presented will focus on the major proposed outline elements (Summary, Preface, Table of Contents, List of Illustrations are straightforward and will not be discussed.) First the purpose and content of each element's final documentation will be discussed. Second, the status of the existing documentation and code (section 1) relating to the final outline element is given. Finally, the actions we will take to complete the documentation are detailed.

The numbering is consistent with the numbering in section B. Section C-1 can be used as a handy guide to major conclusions.

TECHNICAL VOLUME - CHEMFLUB

(Section I) INTRODUCTION

Purpose

A discussion of the models along with their implementation in CHEMFLUB will be discussed. Standard references will be stated, along with assumptions and all necessary arguments which clarify the model's applicability to two-phase reactive flow problems. Also, an overview of the numerical procedures and their applications to the relevant partial and ordinary differential equations will be presented.

Status

The new introduction must track the new document.

Action Required

This will be written in the last phase of document preparation, and will be consistent with the methodology and computer code.

(Section II-1) Governing Equations

(Section II-1.a) Fluids

Purpose of Section

In this section, the system of equations describing the fluid, i.e. gas, will be discussed. These equations relate to mass, momentum, and energy conservation. The differential equations will be presented using the symbolism that will be used in the subsequent numerical development. References to articles that illustrate the development of the equations will be given for the interested reader. Also, the associated initial and boundary conditions will be stated. Thus, this subsection will present a well-posed mathematical model, including boundary and initial conditions.

Status

The fluid equations are presently described in Volume II, Section 3.1, of Systems, Sciences, and Software's technical report. These differential equations are correct and are acceptable. However, the form of these equations is not specifically stated as being those the same as used in the code.

Actions Required

We will cast the equations in the same form as used in the code. The boundary and initial conditions will be reconstructed from the code. Exercising of the code will be necessary to verify that the boundary and initial conditions are correctly posed.

(Section II-1.b) Particles

Purpose of Section

CHEMFLUB models particles as a fluid, thus the differential equations and boundary conditions will be treated similarly to the fluids equations described previously.

Status

The "fluid" equations representing the particles are described in Volume II, Section 3.1; however, many constants used in this formulation are not explicitly defined. Examples being the constants incorporated in equations 3.6 and 3.8b. Examination of the solid pressure term shows the model to be consistent with the formulation of Pritchett et al. and is basically acceptable.

Actions Required

The equations will be cast in the same form as used in the code. The boundary and initial conditions will be reconstructed from the code.

(Section II-2) Chemistry

(Section II-2a) Homogeneous Chemistry

Purpose of Section

This section will clearly state the underlying assumptions made in modeling the chemistry process. It will: 1) enumerate the chemical reactions and the kinetic mechanisms (expressions) for the reactions, 2) present clearly defined and referenced values for the parameters used in the kinetic expressions, and 3) describe the limitations of the model.

Status

The chemistry documentation is presented in Vol. II, Section 3.1. The treatment is basically acceptable, with the exception of the rate constant implicitly incorporated in "gamma" of equation 3.R1. Also, this chemistry model neglects the gas phase oxidation of hydrogen and methane.

Actions Required

The constants described above will be taken from the code and included in the documentation. References will be found for these constants. Reactions which occur in an oxygen rich system will be included.

(Section II-2b) Heterogeneous Kinetics

Purpose of Section

This subsection will be identical to the prior subsection in format; however, in content the models, differential equations, and rate constants will pertain to the heterogeneous chemical reactions.

Status

The chemistry documentation is presented in Volume II, Section 3.1. The treatment is basically acceptable, with the exception of some constants necessary for the evaluation of the rate constant R_i (rate of carbon mass loss per unit surface area). Specifically, equations 3.12b and 3.12c, incorporate unknown constants D_O and D_{OE}.

Action Required

The model will be referenced and the rate constants will be evaluated via a line by line examination of the chemistry subroutines of CHEMFLUB.

(Section II-3) Closure Equations

(Section II-3a) Laminar Model

Purpose of Section

This section will present the semi-empirical model used in this program.

Status

The semi-empirical model is presented in Volume II, Section III-3.1. This formulation is highly questionable. Many of the constants required for this model are not stated or referenced in the documentation.

Actions Required

The constants needed for the documentation will be obtained from the code and verified by use of references obtained through Task 3.1. The entire methodology will be examined for its validity to coal gasifiers via comparisons with test cases.

(Section II-3B) Turbulent Model

Purpose of Section

This section will present the empirical model used for turbulent viscosity in this program.

Status

The empirical model used here is in Volume II, Section III-3.1. This formulation is highly questionable. Many of the constants required for this model are not included in the documentation.

Actions Required

The remaining constants needed for the documentation will be obtained from the code and verified by use of referenced obtained through Task 3.1. The entire methodology will be examined for its validity to coal gasifiers via comparisons with test cases.

(Section II-3c) Drag Coefficient Model

Purpose of Section

The Pritchett model of the velocity-dependent force between the particles and gas constituents will be presented in this section.

Status

The drag coefficient model derived by Pritchett et. al. is in Volume II, Section III-3.1 of the original documentation. The treatment needs to be reorganized and the inherent assumptions and limitations clearly stated.

Actions Required

This section will be reorganized, with the assumptions and limitations included.

(Section II-4) Radiation

Purpose of Section

This section will present the energy transport model.

Status

The existing documentation in Volume II, Section III-3.1 is acceptable. This is a standard formulation.

Actions Required

Documentation is complete, except for the specific value of the thermal diffusion coefficient. Of course, proper implementation of this model in the code will be checked as the code is exercised.

(Section III) - GRID

Purpose of Section

This section will address the numerical grid generation. Establishment of the grid upon which the numerical difference equations are based will be discussed. Issues such as the relationship between the boundary conditions of the physical reactor vessel and the numerical grid approximation will be presented.

Status

A brief, one sentence statement refers to the grid in Volume II, Section III-3.2.

Actions Required

This section must be developed. The existing techniques will be determined from a line by line reconstruction from the code.

(Section IV) Method of Solution
(Section IV-1) Differences Formula

Purpose of Section

This subsection will present a well-posed mathematical problem by including the differenced equation system, as well as the associated differenced boundary conditions and initial conditions. These equations will be given in the form in which they are implemented in CHEMFLUB facilitating future modifications.

Status

There is no documentation of the difference formula. General descriptions such as, "The model involves a combined Eulerian-Lagrangian formulation...." is not helpful unless some specifics are given.

In this section, one expects to find concrete methodologies. Also, the flow charts given are not complete and only hint at the solution.

Actions Required

The difference formula will be reconstructred from the code itself.

(Section IV-2) Stability and Convergence Criteria

Purpose of Section

This section will document stability and convergence criteria, i.e., the relationships between spatial and temporal numerical increments which allow for accurate integration of the difference formula.

Status

There is no documentation of stability and convergence criteria.

Actions Required

The difference formula will be reconstructed from the code itself.

(Section IV-3) Solution Algorithms

Purpose of Section

This section will present a complete set of solution algorithms for each subset of the total equation system. For example, this section will include examples of how to numerically handle singularities at r=0. These algorithms will be described in easily followed flow charts.

Status

Only partial documentation is presented in Volume II, Section III-3.2. The flow charts are not complete and only hint at the solution algorithms.

Actions Required

The complete set of solution algorithms need to be developed. Existing documentation will be used where it exists. The remainder will be reconstructed from the code.

(Section IV-4) Generalized Solution Techniques

Purpose of Section

This subsection will present a coherent picture of how many individual algorithms are linked to form one generalized solution technique which integrates the relevant system of equations.

Status

Some documentation exists in Volume II, Section III-3.2. This consists of one flow chart and a few lines of text. This is not useful because it is too vague.

Actions Required

The complete solution technique needs to be reconstructed. We will do this from the code.

USER'S MANUAL - CHEMFLUB

(Section I) Introduction

Purpose of Section

This section will present a description of the User's Manual's structure.

Status

The new introduction must track the new document.

Actions Required

This will be written in the last phase of document preparation.

(Section II) Description of Input/Output Variables

Purpose of Section

All relevant variables necessary to run the computer code will be explained. Also, incorporated and discussed in this section will be the output variables generated during the execution of the code. This section will contain enough clarity so that the reader will not have to refer to the technical volume to comprehend the variable's function.

Status

The existing documentation in Volume III, Sections 3.4 and 5.0 is incomplete. For example, a complete, easily comprehended section relating to input parameters is missing.

Actions Required

This section needs to be rewritten, with missing sections of the documentation filled in from the code.

(Section III) Input Guide

Purpose of Section

This section will present all necessary information needed to run the computer code. Also, various options available to the user will be explicitly discussed.

Examples of the kind of information which will be included are: (1) how to modify the mesh structure, (2) options on printing output variables, (3) use of graphics (if incorporated) and (4) discussion of restart capabilities.

Status

The present input guide in Volume III, Section 5 is incomplete and does not allow the user to easily run computer cases. For example, the sample case that is given is difficult to input, since the form is so restrictive to formatting procedures.

Actions Required

This section will be rewritten using the existing documentation as well as information reconstructed from the code.

(Section IV) Input/Output Files

Purpose of Section

This section will discuss the nature of the input and output files, i.e. formatting, names, memory sizes.

Status

No explicit description of Input/Output files is given in the present documentation.

Actions Required

This section needs to be developed. The subsequent discussion will be based on experience and the final form of the CHEMFLUB computer code.

(Section V) <u>Flow chart</u>

<u>Purpose of Section</u>

This section will present a detailed flow chart of the computer code.

The structure of the computer code will also be discussed in this section with additional comment statements incorporated in the computer code to allow the user to easily identify the calculations being performed with the numerical model discussed in the technical report.

<u>Status</u>

No detaled flow charts are given on the present documentation of CHEMFLUB.

<u>Actions Required</u>

A flow chart which represent the final configuration of the code must be developed.

(Section VI) Diagnostic Messages

Purpose of Section

This section will discuss diagnostic comments, error messages, etc. to be incorporated in the computer code which aid the user.

Checks of inconsistencies in input conditions, time step requirements, development of instabilities, etc., will be incorporated in the computer code, as well as messages printed to inform the user of potential problems.

Status

Diagnostic messages are not explicitly stated in the documentation.

Actions Required

These messages will be added where appropriate as the program progresses.

(Section VII) Sample Cases

Purpose of Section

In this section, sample cases will be presented to allow a new user to verify that the computer code is running properly. The case being exercised will first be discussed. Also, a listing of the input will be shown and with its generated output. By presenting sample cases in this manner, the user can independently establish his own input file and then compare it with the sample input file to verify that he is correctly following the input guide in Section III. Also, the user can compare the results with the sample output. Cases will be presented for both cold and restart cases.

The sample cases will show all of the required job control language information.

Status

A sample case is presented in Volume III, Appendix A. What was presented is acceptable, except that too much output is included.

Actions Required

The actual sample cases incorporated will be cases run during the performance of Tasks 3.3 - 3.7.

Only that information which is necessary to convince a new user that he has exercised CHEMFLUB successfully will be included.

(Section VIII) General Comments and Observations

Purpose of Section

Within this section general comments and observations will be made regarding the execution and application of the computer code. During the performance of tasks in this program information will be obtained which will be beneficial to other users. This section is structured in order to make this information available to them. It will include helpful comments on observed limitations, suggested input variables, etc. This information is not available in the present documentation.

Status

No such section exists in the present documentation.

Actions Required

This section will be developed.

D. RECOMMENDED PLAN TO COMPLETE DOCUMENTATION

1) Discussion

a) Reconstruction of Documentation

The lack of documentation of numerical techniques is unacceptable and must be corrected before the exercise tasks can be properly carried out. While the code runs and provides output, it is useless to proceed without the ability for independent verification of the numerics. We therefore purpose to reconstruct the numerical algorithms by a line by line examination of the code and by exercising specific code sections. Additional reconstruction or rewriting needed in other documentation sections is presented in the text of this report. However, the absence of numerics is considered the most serious situation.

As shown in figure 6, the reconstruction activity will be scheduled over the next 4 month period. This reconstruction activity may identify code modifications that are necessary and which would be performed under of Task 3.6, Modification of Models/Codes. The reconstruction of the documentation will result in a baseline for further improvements and modifications.

b) Final Documentation

The documentation will be presented in three volumes. Volume I will cover technical issues, Volume II will be a user's manual and Volume III will be a systems manual. The outline of each volume is presented in section B. In addition, an extensive appendix of relevant reference material will be either included with the Technical Volume or presented separately.

c) Documentation Input

The reconstruction described above will provide the base revised documentation material. As the program proceeds, input material will be generated in the code exercise tasks (3.3, 3.4, 3.5). Experience with system files, necessary default options, etc., are some of the types of documentation input we will gain from these tasks. Modifications approved under Task 3.6 will form a second source of revisions for both the documentation and the code itself.

2) Schedule

The necessary reconstruction of the documentation is scheduled for a 4 month period, as shown in figure 6. To avoid a seve impact on the scheduled exercising of the code in Task 3.3, we will stage the documentation reconstruction activity. First, we will reconstruct the gas fluid algorithms. This can then be used in exercising some of standard flow conditions in Task 3.3a appropriate for CHEMFLUB. The particle-fluid algorithms will be treated next, followed by the chemistry algorithms. The dotted line labeled 1 in figure 6 denotes this interaction between reconstruction and exercising activity. The line labeled 2, denotes modifications that may be necessary because of information developed during the reconstruction.

Changes in the code or documentation that are found to be necessary during performance of Task 3.3, as well as Tasks 3.4, 3.5, and 3.7, will be made under Task 3.6 and included in the documentation as illustrated by the dotted line 4 in figure 6. Other changes that are found to be necessary will be made in Task 3.6 and included in the documentation.

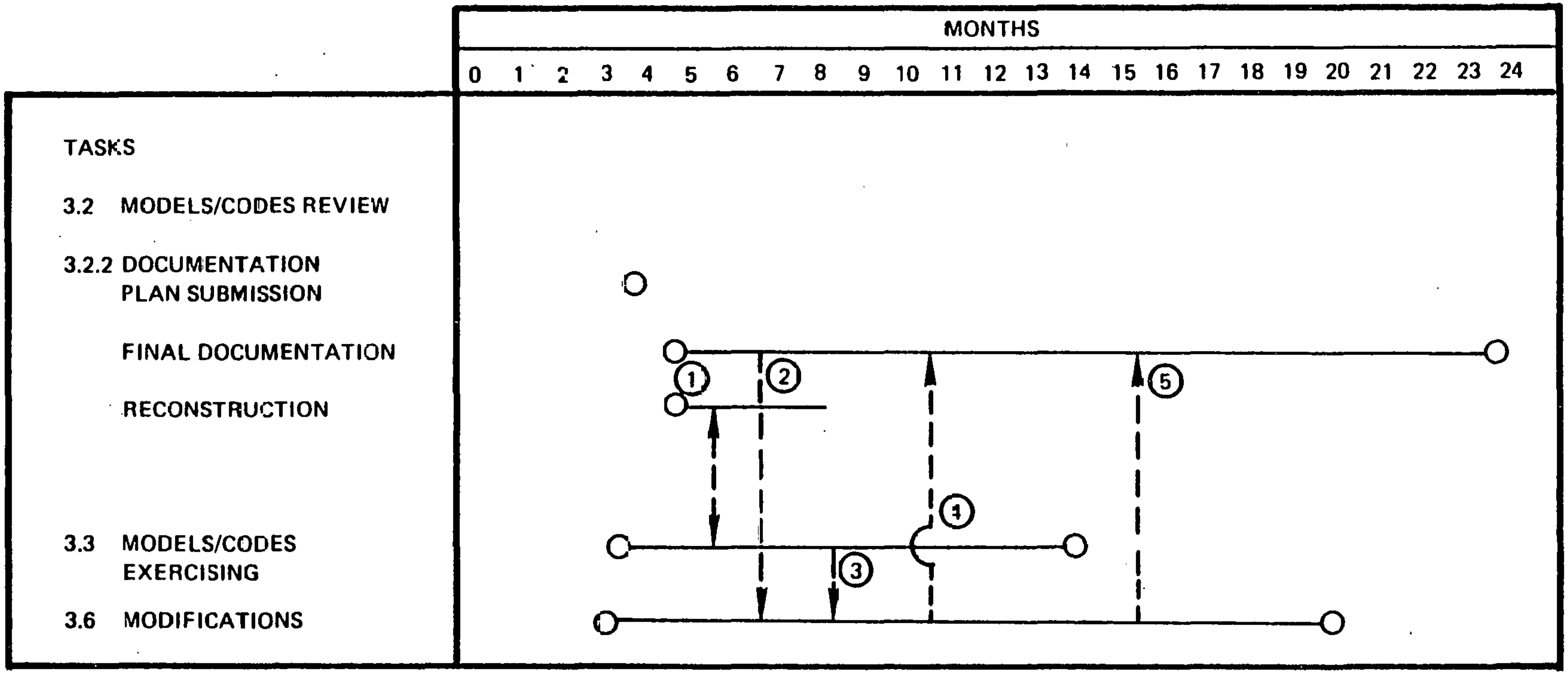
3) Communication and Logging of Modifications

a) Regarding Documentation

The present plan devotes a separate page and discussion to each major section of the final documentation. This format will be converted into a loose leaf set of volumes. As sections of the documentation are reconstructed they will be inserted in the loose leaf folders. The same volumes can be updated as additional sections are rewritten or updated. A separate volume will collect material that is replaced. Separate sets of volumes will be kept at METC, BDM and Exxon. The monthly technical progress report will be the vehicle for transmitting sections of the documentation.

b) Code Modifications and Transmission of Modifications

Two separate copies of each code (CHEMFLUB and FLAG) will reside on the BDM-VAX computer system in Washington, D.C. One copy will only be accessed by one user responsible for both updating and



(1) RECONSTRUCTION PROCEEDS WITH CONCURRENT EXERCISING

(2) MODIFICATIONS OF THE CODE MAY BE NECESSARY AND WILL BE DONE UNDER TASK 3.6

(3) MODIFICATIONS NEEDED AND IDENTIFIED DURING EXERCISING WILL BE DONE UNDER TASKS 3.6

(4) MODIFICATIONS WILL BE INCLUDED IN DOCUMENTATION UPON APPROVAL BY DOE

(5) FURTHER MODIFICATIONS WILL BE REQUIRED AS A RESULT OF TASKS 3.4 AND 3.5

Figure 6. Schedule - CHEMFLUB

documenting changes to this copy. The record of the alterations and modifications will be done via comment statements in the code and a written log stating the changes. The other copy will be a working copy of the updated code accessed by all users. As problems are successfully addressed the required modifications will be given to the one user responsible for the one copy which is used only for documentation. Only this person will update the documented version. This allows for a sample path of information flow.

On a monthly basis, the changes for each code will be transmitted to METC along with a copy of the associated written log. This procedure after the next 4 months (reconstruction period) will be done on a quarterly basis.

c) Technical Communication

It is strongly recommended that METC interact with BDM on two levels. First, METC technical staff should come to Albuquerque and spend a period of time consistent with their learning about our technical plans and the resulting required actions. Second, METC should link to the BDM-VAX in Washington, D.C. to facilitate the monthly transfer of the changes.

VOLUME III
SYSTEMS MANUAL

The purpose of the Systems Manual Volume is to provide detailed material and descriptions relating to the structure and operation of the computer code. It is prepared for computer scientists, systems level analysts, and programmers whose responsibilities are major modifications to the computer code, transfering the computer code to other operating systems, resolution of program/system problems, etc. This volume is not being written for the physicists or engineering users of the computer code. The Technical and User's Volumes will be prepared for these individuals.

PREFACE

This section will discuss the purpose of this volume. Reference will be made to the Contracting Agency and Contract Number.

I. INTRODUCTION

The purpose of this section is to discuss the structure of this volume.

II. FUNDAMENTALS

This section will discuss the overall philosophy of the structure of the code. This will include hardware considerations, handling of input/output files, restart considerations and diagnostic messages which are system specific. This section will serve as a general background for the remainder of this volume.

III. DATA BLOCKS

This section will present the data blocks incorporated in the code (i.e., common blocks, equivalenced data, initilization data, parameter statements, etc.) as well as an explanation of the variables.

IV. MODULES

This section will discuss the modules which comprise the code. The function of each of the modules will also be discussed.

V. SUBROUTINES

This section will address the subroutines which comprise each of the modules. The utility subroutines will also be addressed in this section .

VI OPERATIONAL SYSTEM INTERFACES

This section will discuss the job control language necessary for executing the computer code.

VII CODE MODIFICATIONS/ADDITIONS

This section will discuss how the computer code can be modified and how these changes are implemented.