DOCKET NO. 50—245
LICENSE NO. DPR—21

MILLSTONE UNIT NO. I
Combustible Gas Control Evaluation

NORTHEAST UTILITIES

THE CONNECTICUT LIGHT AND POWER COMPANY
THE HARTFORD ELECTRIC LIGHT COMPANY
WESTERN MASSACHUSETTS ELECTRIC COMPANY
HOLYOKE WATER POWER COMPANY
NORTHEAST UTILITIES SERVICE COMPANY
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August 6, 1982

Docket No. 50-245
B10533

Mr. William J. Dircks
Executive Director for Operations
U. S. Nuclear Regulatory Commission
Washington, D. C. 20555

References:

(1) W. G. Counsil letter to W. J. Dircks, dated January 26, 1982.

(2) W. G. Counsil letter to W. J. Dircks, dated April 2, 1982.

(3) W. Gammill letter to W. G. Counsil, dated August 27, 1979.

(4) D. L. Ziemann letter to W. G. Counsil, dated April 18, 1980.

(5) W. C. Counsil letter to D. L. Ziemann, dated November 28, 1979.

(6) G. C. Lainas letter to All SEP Licensees, dated May 7, 1981.

(7) W. C. Counsil letter to W. J. Dircks, dated December 28, 1981.

Gentlemen:

Millstone Nuclear Power Station, Unit No. 1
Combustible Gas Control Evaluation

In Reference (1), Northeast Nuclear Energy Company (NNECO) informed the NRC Staff that since the requirement for hydrogen recombiner capability was not known to us until the promulgation of the December 2, 1981 final rule on "Interim Requirements Related to Hydrogen Control," we had not yet been able to determine whether the requirement for such capability is technically justified for Millstone Unit No. 1. Furthermore, we indicated that we intended to submit our conclusions on this topic within approximately two (2) months. The results of our preliminary evaluation and the status of our analyses still in progress at that time were submitted in Reference (2).

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1/35

Our preliminary results showed that the actual extent of net radiolysis is substantially less than that required to obtain a flammable gas mixture inside primary containment, the generation and control of post-accident oxygen is the dominant concern in an inerted containment, and large amounts of metal-water reactions tend to make the primary containment more inert since under inerted conditions hydrogen acts as an oxygen diluent. Subject to additional analysis and verification, we concluded that only an inerted containment at Millstone Unit No. 1 is necessary to adequately preclude the formation of a flammable gas mixture inside primary containment following a design basis LOCA. This conclusion results in a situation where neither venting of the containment, post-accident nitrogen addition, nor hydrogen recombiners are required as a means of combustible gas control following a design basis LOCA.

We also indicated in Reference (2) that by July 1, 1982 we intended to finalize our preliminary results and establish a schedule for implementation of plant modifications necessary to convert MSIV and S/RV control air to nitrogen in order to eliminate the dominant post-accident oxygen source. On June 18, 1982, we contacted the NRC Project Manager for Millstone Unit No. 1 and informed him that our July 1, 1982 submittal would be delayed. Therefore, the purpose of this submittal is to provide the results of our evaluation, submit our conclusions regarding the provisions of 10CFR50.44 in its entirety, and inform you of our current schedule to implement those plant modifications necessary to convert control air to nitrogen during our next refueling outage. Based on our plans to convert control air to nitrogen, post-accident air leakage from the MSIVs and S/RVs is not considered a potential oxygen source in our evaluation.

A detailed technical description of our evaluation and our findings can be found in the attachments. Our evaluation consists primarily of determining preaccident initial gas concentrations within the Millstone Unit No. 1 nitrogen inerted containment, the extent of short-term generation of hydrogen and oxygen from various values of metal-water reactions and boiling phase radiolysis, and the extent of long-term generation of hydrogen and oxygen from non-boiling phase radiolysis. The hydrogen and oxygen concentrations inside containment that result from our consideration of metal-water reactions and both boiling and non-boiling phases of radiolysis are then compared with the flammability limits for hydrogen and oxygen. The non-boiling phase radiolysis accounts for the very significant recombination effects in pure and contaminated water at different water temperatures, volumetric flow rates through the core, and initial hydrogen and oxygen concentrations. Our consideration of the inherent natural recombination of hydrogen and oxygen is the major difference between our model and that which is identified in Regulatory Guide 1.7.

In most cases, equilibrium is reached shortly after cessation of boiling such that no additional net hydrogen and oxygen is produced. In fact, in many cases the hydrogen and oxygen concentrations in the primary containment are actually shown to decrease after boiling ceases. For metal-water reactions greater than approximately 0.2%, the reactor coolant is stable against any further net radiolysis at the time boiling ceases. For metal water reactions less than approximately 0.2%, there may be some additional net radiolysis if high levels of impurities are postulated until the dissolved hydrogen level in the coolant increases to a level where equilibrium between radiolytic decomposition and recombination is achieved. In either case, the peak hydrogen and oxygen concentrations predicted are less than the flammability limits.

The most limiting range of metal-water reactions is for very small reactions (i.e., less than 1%). It is important to note that a 0.19% metal-water reaction is postulated for a design basis LOCA. 10CFR50.44(d)(1) requires that five (5) times this value, or approximately 1%, be assumed. Therefore, the most limiting cases are actually within the design basis of Millstone Unit No. 1. Metal-water reactions beyond 1% would reduce flammability concerns since the additional hydrogen proportionally reduces the oxygen concentration inside the primary containment and yields a more inert condition.

The attached evaluation illustrates that the impact of chemical and fission product impurities on the recombination effect is insufficient to produce flammable mixtures. The fundamental basis for treating fission product impurities is the knowledge that a significant fission product release to the coolant water can only occur if extensive fuel damage (substantially beyond the design basis LOCA) is postulated. Such fuel damage necessarily implies an appreciable amount of metal-water reaction and therefore evolution of excess hydrogen gas. This excess hydrogen gas significantly promotes recombination and also reduces the oxygen concentration inside the primary containment.

The most significant conclusion resulting from the attached evaluation, which fully supports our preliminary evaluation submitted in Reference (2), is that an inerted containment at Millstone Unit No. 1 is sufficient by itself to preclude the formation of a flammable gas mixture for an indefinite period without the need for either containment purging, post-accident nitrogen addition, or hydrogen recombiners. Our evaluation has demonstrated that one of the key physical features for assuring combustible gas control is the existence in all cases of a hydrogen gas overpressure in the containment. This hydrogen gas overpressure assures a dissolved hydrogen concentration in coolant liquids which is sufficient to stabilize radiolysis, but is insufficient to become flammable.

In assessing the potential benefits of hydrogen recombiners, it is significantly noted that the removal of the hydrogen and oxygen gas from the containment by a hydrogen recombiner will reduce the overpressure these gases exert on the reactor coolant water. The reduction of this overpressure decreases hydrogen and oxygen gas solubility in the coolant water, which causes more hydrogen and oxygen gas to enter the containment gas region and reduces the dissolved gas concentrations in the coolant. If a substantial reduction in dissolved hydrogen gas concentration occurs, net radiolysis and generation of more hydrogen and oxygen gas will ensue in an attempt to restore the equilibrium balance. Therefore, the potential benefits of hydrogen recombiners in an inerted containment may be mitigated by the natural processes taking place in a post-LOCA environment.

Independent review of selected portions of our evaluation by personnel of the Argonne National Laboratory, AERE/Harwell in the United Kingdom, General Electric, and Northeast Utilities Service Company (NUSCO) is ongoing. Upon completion of such review, the NRC Staff will be informed.

Before discussing the status of our compliance with 10CFR50.44, it is appropriate to briefly review the licensing chronology included as Attachment No. 1. The attached chronology illustrates the substantial amount of information that has been transmitted between the NRC and NNECO over the past several years regarding combustible gas control at Millstone Unit No. 1. The chronology shows that combustible gas control at Millstone Unit No. 1 was being addressed by the NRC and NNECO long before the first version of 10CFR50.44 was published as final in the Federal Register on October 27, 1978. The chronology also demonstrates our responsiveness to NRC concerns on this issue as well as our determination to adequately resolve this problem.

It appears that the most significant impact of the promulgation of the October 27, 1978 version of 10CFR50.44 upon NNECO was that final regulations existed which would then have allowed an Air Containment Atmospheric Dilution (ACAD) system to be utilized for combustible gas control and deinerting of the containment. To the best of our ability, we have been unable to determine any implementation date for the October 27, 1978 version of 10CFR50.44. Although 10CFR50.44 was published on October 27, 1978 and became effective on November 27, 1978, it hardly seems reasonable to assume that the NRC intended licensees to comply with this regulation within thirty (30) days. Therefore, the record shows we were continuing our efforts to submit to the NRC final design details of our ACAD system when the TMI-2 incident occurred.

Subsequent to TMI-2, we received correspondence from the NRC (Reference (3)) informing us that any further NRC review work on our ACAD system and deinerting submittals was being suspended until the Commission acted on the TMI-2 Lessons Learned Task Group's recommendations. This letter specifically states that we would "be informed when the Commission acts and of the impact on your request." Reference (3) could be interpreted such that implementation of any modifications to the then-current combustible gas control systems was no longer required until so informed by the NRC.

NNECO has responded to all NRC post-TMI items regarding combustible gas control systems. Additionally, in Reference (4) we received confirmation that all of our responses were acceptable to the NRC. One item (NUREG-0578, Item 2.1.5a) was deferred to Systemmatic Evaluation Program (SEP) Topic VI-5, "Combustible Gas Control." NNECO provided a significant amount of information in response to NRC questions on this topic in Reference (5). The then-current method of combustible gas control at Millstone Unit No. 1 was described in detail in that submittal. Additionally, specific requirements of then-current 10CFR50.44 were addressed.

In Reference (6), SEP Topic VI-5 was deleted from the SEP on the basis of TMI Item II.B.7 and USI A-48. TMI Item II.B.7 involves short-term and long-term rulemaking to amend 10CFR50.44. The final rule on "Interium Requirements Related to Hydrogen Control," dated December 2, 1981, represents such short-term rulemaking. Long-term rulemaking is currently in progress (i.e., the proposed rule dated December 23, 1981). Therefore, correspondence identified in Attachment No. 1 leads one to conclude that we are now required to address all the requirements of 10CFR50.44 as it exists as of January 4, 1982. References (1), (2), and (7) were previously submitted specifically in response to the final rule published in the Federal Register on December 2, 1981.

In conclusion, the attached evaluation demonstrates that the primary means of combustible gas control at Millstone Unit No. 1 is a nitrogen inerted containment. Additionally, containment purging, post-accident nitrogen addition, and hydrogen recombiners are not necessary for combustible gas control following a design basis LOCA. Based on these results and our plans to convert MSIV and S/RV control air to nitrogen during the next refueling outage, we conclude that we will be in full compliance with 10CFR50.44 in its entirety by the end of our next refueling outage. This schedule is fully consistent with the schedule required by 10CFR50.44. A detailed illustration of such compliance can be found in Attachment No. 2. Therefore, requests for exemptions from any portion of 10CFR50.44 are not necessary.

We are willing to meet with you to discuss any questions you may have regarding this submittal.

Very truly yours,

NORTHEAST NUCLEAR ENERGY COMPANY
NORTHEAST UTILITIES SERVICE COMPANY

W. G. Counsil

W. G. Counsil
Senior Vice President

J. P. Cagnetta

By: J. P. Cagnetta
Vice President
Nuclear and Environmental Engineering

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ATTACHMENTS

MILLSTONE NUCLEAR POWER STATION, UNIT NO. 1

COMBUSTIBLE GAS CONTROL EVALUATION

AUGUST, 1982

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MILLSTONE NUCLEAR POWER STATION, UNIT NO. 1

COMBUSTIBLE GAS CONTROL EVALUATION

AUGUST, 1982

MILLSTONE UNIT NO. 1
COMBUSTIBLE GAS CONTROL
LICENSING CHRONOLOGY

1. JANUARY 1970:

Information was presented at the January 1970 ACRS meeting regarding the radiological consequences of hydrogen generation post-LOCA. Formal submission of such information was subsequently made by referencing the Dresden Nuclear Power Station Unit 3, Amendment 23, "Hydrogen Generation in a Boiling Water Reactor." Based upon the referenced analyses, one could conclude that the radiological consequences of containment venting are inconsequential compared to the radiation dose received from normal containment leakage if realistic values for the metal-water reaction and radiolytic hydrogen production are assumed.

2. MARCH 10, 1971:

Atomic Energy Commission (AEC) published Safety Guide 7 which provided guidance to be used in evaluating the consequences of hydrogen generation following a LOCA.

3. OCTOBER 13, 1971:

AEC (Dr. Peter Morris) letter requested Millstone Point Company (MPC) to address the consequences of hydrogen and oxygen generation following a LOCA based upon the parameters listed in Table 1 of Safety Guide 7, which included an assumption of 5% metal-water reaction.

4. APRIL 28, 1972:

In response to the AEC letter dated 10/13/71, the MPC (subsequently changed to NNECO) submitted a detailed analysis based upon the assumptions in Safety Guide 7. The MPC proposed adding nitrogen to the containment to maintain oxygen concentrations below the 5% limit. The analysis indicated that it would take at least 40 days following a LOCA before 50% of the containment design pressure is attained assuming zero containment leakage. If containment leakage is 20% or greater than that allowed by the Technical Specifications, no containment venting would be required. If the containment were vented after one month under average meteorological conditions the resulting incremental radiation dose (thyroid dose controlling value) to any individual beyond the site boundary would be approximately 1% of those exposures reported in the AEC Safety Evaluation for Millstone due to containment leakage following a LOCA, and about 2% of the incremental dose guideline stated in the AEC October 1971 letter. Therefore, MPC believed that the nitrogen addition concept provided a satisfactory alternative to containment purging.

5. SEPTEMBER 1, 1972:

MPC submitted a FTOL application. Section 7.2 of this application addressed hydrogen control post-LOCA and was essentially identical to the analysis provided in our April 28, 1972 submittal.

6. JUNE 22, 1973:

Question #6 of AEC letter (D. L. Ziemann) requested additional information regarding containment atmospheric dilution system including P&IDs and other details.

7. JANUARY 24, 1974:

Appendix B to FTOL application was submitted which addressed Question #6 in AEC's letter dated 6/22/73. A significant amount of information regarding a nitrogen supplying containment atmospheric dilution (CAD) system was provided.

8. MAY 29, 1974:

NUSCO submitted comments on proposed Revision 1 of Regulatory Guide 1.7. NUSCO indicated that the high degree of conservatism in Regulatory Guide 1.7 results in unnecessary design margin in the equipment provided to control the combustible gases following a postulated loss of coolant accident. Additionally, the operation of many boiling water reactors would be burdened unnecessarily by the wording of this Guide. The proposed revision fails to reduce conservatism to a level which provides realistic margin. In several specific instances, such a reduction to achieve realistic margins would not compromise nuclear safety.

9. SEPTEMBER 19, 1974:

To continue its review of MPC's FTOL application, the AEC requested additional information (Question #3) on the CAD system including details of the oxygen monitoring system.

10. OCTOBER 18, 1974:

NNECO submitted Appendix F to FTOL application which responded to AEC's 9/19/74 letter.

11. FEBRUARY 19, 1975:

NRC (G. Lear) letter requesting additional information concerning the proposed CAD system.

12. MARCH 21, 1975:

NNECO responded to NRC letter dated 2/19/75. This submittal included proposed technical specfication changes to limit oxygen concentration to be less than 4% by volume during normal operation. Design details regarding the oxygen monitoring system were also provided. NNECO again noted the proposed design was based upon then current regulatory criteria and that, therefore, the proposed CAD system was subject to modification upon revisions in regulatory criteria.

13. SEPTEMBER 1976:

Revision 1 to Regulatory Guide 1.7, which replaced Safety Guide 7, was published for comment.

14. OCTOBER 21, 1976:

NRC published the notice of proposed rule making in 41 FR 46167 for 10CFR50.44. This allowed for repressurization (nitrogen or air) as a primary means of combustible gas control in plants of Millstone's vintage.

15. JANUARY 1977:

Based on Revision 1 to Regulatory Guide 1.7 and proposed 10CFR50.44, a "Combustible Gas Control System Design Report" was prepared describing an Air Containment Atmospheric Dilution (ACAD) system. This report was planned to be submitted upon finalization of rulemaking on 10CFR50.44. The combustible gas control system described in this report was designed in accordance with guidelines contained in Branch Technical Position CSB 6-2, "Control of Combustible Gas Concentrations in Containment Following a Loss-of-Coolant Accident." The system was also designed in accordance with GDC 41, 42, and 43. Additionally, the system would control combustible gas concentrations with a minimum release of radioactive effluent to the environment. The resulting doses would have been a fraction of 10CFR100 regulations.

16. OCTOBER 27, 1978:

Final rule on 10CFR50.44 published in Federal Register with an effective date of November 27, 1978. A schedule for implementation of this final rule was not provided in the Federal Register notice. It appears that the most significant impact of the promulgation of 10CFR50.44 upon NNECO was that final regulations existed which would allow an Air Containment Atmospheric Dilution (ACAD) system to be utilized for combustible gas control and deinerting of the containment. Therefore, it is arguable that if a licensee had wished to maintain an inerted containment, such inerting would constitute the primary means of combustible gas control and automatic compliance with 10CFR50.44.

17. NOVEMBER 1978:

Revision 2 to Regulatory Guide 1.7 was published. This revision was essentially the same as Revision 1 but referenced the final 10CFR50.44.

18. MARCH 28, 1979:

TMI-2 incident.

19. AUGUST 27, 1979:

NRC letter (W. Gammill) suspending any further review work on NNECO's CAD system and deinerting submittals until the Commission acted on the TMI-2 Lessons Learned Task Group's recommendations. This letter specifically stated that we would "be informed when the Commission acts and of the impact on your request." The NRC's letter could be interpreted to imply that implementation of any modifications to the then-current combustible gas control systems was no longer required until so informed by the NRC.

20. SEPTEMBER 13, 1979

NRC (D. G. Eisenhut) letter to All Operating Nuclear Power Plants requesting implementation of NUREG-0578. Of particular interest were Items 2.1.5.a,b, and c.

21. OCTOBER 18, 1979:

W. G. Counsil letter to D. G. Eisenhut responding to NRC's 9/13/79 letter.

Post-Accident Hydrogen Control Systems for PWR and BWR Containments

2.1.5.a

a. Dedicated Penetrations for External Recombiner or Post-Accident External Purge System

NNECO Response

The actions required for this item will be integrated within the Systematic Evaluation Program (SEP) under the topic "Combustible Gas Control" (Topic VI-5).

2.1.5.b & c

b. Inerting BWR Containments

c. Capability to Install Hydrogen Recombiner at Each Light Water Nuclear Power Plant

NNECO Response

These items have been deferred for evaluation by the NRC.

22. NOVEMBER 28, 1979:

W. G. Counsil (NNECO) letter to D. L. Ziemann on SEP Topic VI-5, "Combustible Gas Control". This letter responded to questions informally received from the NRC staff.

The current method of combustible gas control at Millstone Unit No. 1 was described in detail in this submittal. The references for SEP Topic VI-5 include 10CFR50.44, BTP CSB6-2, SRP 6.2.5, and DOR Technical Activities, Category A, Items 8 and 14. Various 10CFR50.44 requirements were addresssed by NNECO in this submittal.

23. APRIL 18, 1980:

NRC SER for TMI Category A items. NRC concluded that we had satisfactorily met all Category A requirements. Specifically, the NRC Staff's evaluation for Items 2.1.5.a and 2.1.5.c follow:

2.1.5.a Dedicated Penetrations for External Recombiner or Post-Accident External Purge System

The staff's position is that licensees whose plant uses external recombiners or purge systems for post-accident control of combustible gas in the containment atmosphere should provide a penetration that is dedicated to that function only. As stated in our letter dated October 30, 1979, this requirement is applicable to those plant whose licensing basis includes requirements for external or purge systems for post-accident control of combustible gas in the primary containment.

We have determined that this item is not directly applicable to Millstone Unit No. 1. The question of post-accident combustible gas control at Millstone will be reviewed by our ongoing Systematic Evaluation Program, Item VI-5. Therefore, we find that the licensee has satisfied the Category "A" requirements for this item.

2.1.5.c Recombiner Procedures

The NRC requirements for this item apply only to those plants that include hydrogen recombiners as a design basis for licensing. We have determined that this item is not applicable to the Millstone Unit No. 1 Plant.

24. OCTOBER 2, 1980:

Proposed rule on 10CFR50.44.

25. NOVEMBER 17, 1980:

NNECO comments on 10/2/80 proposed rule.

26. MAY 7, 1981:

NRC letter (G. C. Lainas) to All SEP Licensees deleting SEP Topic VI-5. The basis for the deletion was the following:

Basis for Deletion (i.e., related TMI Task, USI or other SEP Topic)

a. TMI Task Action Plan - NUREG-0660 - Task II.B.7, Analysis of Hydrogen Control

As a result of TMI II.B.7, short and long term rulemaking to amend 10CFR50.44 has been initiated. The short term rulemaking (interim rule) requires that all Mark I and Mark II containments be inerted. It also requires that the owners of all plants with other containments perform certain analyses of accident scenarios involving hydrogen releases and furnish the staff with a proposed approach for mitigating these hydrogen releases.

The longer term rulemaking will address both degraded core and melted core issues. In the area of hydrogen control it will prescribe requirements that are appropriate for operating plants as well as for plants under construction.

b. USI A-48, Hydrogen Control Measures and Effects of Hydrogen Burns on Safety Equipment, NUREG-0705

Under USI A-48 a Task Action Plan has been defined and is being developed that encompasses the concerns in the Definition and the Safety Objective of SEP Topic VI-5.

The evaluation required by TMI II.B.7 and USI A-48 is identical to SEP Topic VI-5; therefore, this SEP topic has been deleted.

27. DECEMBER 2, 1981:

Final rule on "Interim Requirements Related to Hydrogen Control" published in Federal Register. The effective date of this rule was January 4, 1982.

28. DECEMBER 23, 1981:

Proposed rule on "Interim Requirements Related to Hydrogen Control" noticed for comment in the Federal Register.

29. DECEMBER 28, 1981:

W. G. Counsil (NNECO) letter to W. J. Dircks (NRC) regarding the manner by which the December 2, 1981 final rule was promulgated. NNECO's concern was that the requirements in the final rule apparently were changed significantly from those in the proposed rule. Specifically, it was NNECO's understanding that the proposed rule did not require hydrogen recombiner capability for Millstone Unit No. 1; whereas, the final rule could be interpreted to require such capability.

30. JANUARY 26, 1982

W. G. Counsil letter to W. J. Dircks informing the NRC Staff that since the requirement for hydrogen recombiner capability was not known to us until the promulgation of the December 2, 1981 final rule on "Interim Requirements Related to Hydrogen Control," we had not yet been able to determine whether the requirement for such capability is technically justified for Millstone Unit No. 1. Furthermore, we indicated that we intended to submit our conclusions on this topic within approximately two (2) months.

31. APRIL 2, 1982:

W. G. Counsil letter to W. J. Dircks submitting the results of a preliminary evaluation and the status of analyses still in progress. Subject to additional analysis and verification, NNECO concluded that only an inerted containment at Millstone Unit No. 1 is necessary to adequately preclude the formation of a flammable gas mixture inside primary containment following a design basis LOCA. This conclusion results in a situation where neither venting of the containment, post-accident nitrogen addition, nor hydrogen recombiners are required as a means of combustible gas control following a design basis LOCA.

32. APRIL 8, 1982:

NNECO submitted comments on the proposed "Interim Requirements Related to Hydrogen Control," dated 12/23/81. NNECO recommended that this rulemaking process be deferred pending completion of several ongoing studies.

33. APRIL 15, 1982:

R. W. Starostecki (NRC) letter to W. G. Counsil transmitting Inspection Report No. 50-245/82-05. This inspection report discusses the status of Millstone Unit No. 1's compliance with 10CFR50.44.

34. MAY 24, 1982:

W. G. Counsil letter to D. M. Crutchfield regarding TMI Action Item II.B.1, "Reactor Coolant System Vents." This letter describes NNECO's compliance with 10CFR50.44(c)(3)(iii).

35. JUNE 4, 1982:

W. G. Counsil letter to D. G. Eisenhut providing information on TMI Action Item II.F.1.6, "Containment Hydrogen Monitor." NNECO indicated that a value-impact evaluation of this TMI item was warranted. One objective of this evaluation would be to determine the proper role of hydrogen monitoring instrumentaion in accident scenarios involving hydrogen generation.

Docket No. 50-245

ATTACHMENT NO. 2

MILLSTONE NUCLEAR POWER STATION, UNIT NO. 1

COMBUSTIBLE GAS CONTROL EVALUATION

AUGUST, 1982

COMPLIANCE WITH 10CFR50.44

SECTION

50.44(a)

REQUIREMENT

Each boiling or pressurized light-water nuclear power reactor fueled with oxide pellets within cylindrical zircaloy cladding, shall, as provided in 10CFR50.44(b) through (d), include means for control of hydrogen gas that may be generated, following a postulated loss-of-coolant accident (LOCA), by (1) metal-water reaction involving the fuel cladding and the reactor coolant, (2) radiolytic decomposition of the reactor coolant, and (3) corrosion of metals.

STATUS OF COMPLIANCE

A nitrogen inerted containment is our means for control of hydrogen gas that may be generated following a design basis LOCA from (1) metal-water reactions involving the fuel cladding and the reactor coolant, (2) radiolytic decomposition of the reactor coolant, and (3) corrosion of metals. In fact, the more hydrogen generated, the more inert the containment becomes and the more flammability concerns are reduced. Furthermore, for inerted containments, flammability concerns center around oxygen generation not hydrogen. See also Sections 50.44(b), (c), and (d), below.

SECTION

50.44(b)

REQUIREMENT

Each boiling or pressurized light-water nuclear power reactor fueled with oxide pellets within cylindrical zircaloy cladding shall be provided with the capability for (1) measuring the hydrogen concentration in the containment, (2) insuring a mixed atmosphere in the containment, and (3) controlling combustible gas concentrations in the containment following a postulated LOCA.

STATUS OF COMPLIANCE

(1) Capability for measuring the hydrogen concentration inside primary containment following a design basis LOCA currently exists by means of our post-Accident Sampling System.
(2) See Section 2.1 in Volume I of Attachment No. 4 and Item Nos. 7 and 22 in Attachment No. 1.
(3) As illustrated in Attachment No. 4, the inerted containment at Millstone Unit No. 1 provides the capability for controlling combustible gas concentrations inside the containment following a design basis LOCA to below flammable limits.

SECTION

50.44(c)(1)

REQUIREMENT

For each boiling or pressurized light-water nuclear power reactor fueled with oxide pellets within cylindrical zircaloy cladding, it shall be shown that during the time period following a postulated LOCA but prior to effective operation of the combustible gas control system, either: (i) an uncontrolled hydrogen-oxygen recombination would not take place in the containment; or (ii) the plant could withstand the consequences of uncontrolled hydrogen-oxygen recombination without loss of safety function.

STATUS OF COMPLIANCE

Not only does Attachment No. 4 show that an uncontrolled hydrogen-oxygen recombination would not take place, but Millstone Unit No. 1 also complies with 10CFR 50.44(c)(2) below.

SECTION

50.44(c)(2)

REQUIREMENT

If the conditions set out in 10CFR50.44(c)(1) cannot be shown, the containment shall be provided with an inerted or an oxygen deficient atmosphere in order to provide protection against hydrogen burning and explosions during the time period specified in 10CFR50.44(c)(1).

STATUS OF COMPLIANCE

Millstone Unit No. 1 is provided with a nitrogen inerted containment atmosphere.

SECTION

50.44(c)(3)(i)

REQUIREMENT

Notwithstanding 10CFR50.44(c)(1) and (c)(2):

> Effective May 4, 1982 or 6 months after initial criticality, whichever is later, an inerted atmosphere shall be provided for each boiling light-water nuclear power reactor with a Mark I or Mark II type containment.

STATUS OF COMPLIANCE

Millstone Unit No. 1 is provided with a nitrogen inerted containment atmosphere.

SECTION

50.44(c)(3)(ii)

REQUIREMENT

Notwithstanding 10CFR50.44(c)(1) and (c)(2):

> By the end of the first scheduled outage beginning after July 5, 1982 and of sufficient duration to permit required modifications, each light-water nuclear power reactor that relies upon a purge/repressurization system as the primary means for controlling combustible gases following a LOCA shall be provided with either an internal recombiner or the capability to install an external recombiner following the start of an accident. The internal or external recombiners must meet the combustible gas control requirements in 10CFR50.44(d). The containment penetrations used for external recombiners must either be:
>
> (A) dedicated to that service only, conform to the requirements of Criteria 54 and 56 of Appendix A to 10CFR50, be designed against postulated single failures for containment isolation purposes, and be sized to satisfy the flow requirements of the external recombiners, or
>
> (B) of a combined design for use by either external recombiners or purge/ repressurization systems and other systems, conform to the requirements of criteria 54 and 56 of Appendix A to 10CFR50, be designed against postulated single failures both for containment isolation purposes and for operation of the external recombiners or purge/repressurization systems, and be sized to satisy the flow requirements of the external recombiners or purge repressurization systems.

STATUS OF COMPLIANCE

As concluded in Attachment No. 4, the primary and only means necessary for controlling combustible gases following a design basis LOCA at Millstone Unit No. 1 is an inerted containment. Millstone Unit No. 1 does not rely upon a purge/repressurization system to control combustible gases following a design basis LOCA. Therefore, this requirement is not applicable to Millstone Unit No. 1.

SECTION

50.44(c)(3)(iii)

REQUIREMENT

Notwithstanding 10CFR50.44(c)(1) and (c)(2):

> To provide improved operational capability to maintain adequate core cooling following an accident by the end of the first scheduled outage beginning after July 1, 1982 and of sufficient duration to permit required modifications, each light-water nuclear power reactor shall be provided with high point vents for the reactor vessel head, and for other systems required to maintain adequate core cooling if the accumulation of noncondensible gases would cause the loss of function of these systems. (High point vents are not required, however, for the tubes in U-tube steam generators.) The high point vents must be remotely operated from the control pressure boundary, the design of the vents and associated controls, instruments and power sources must conform to the requirements of Appendix A and Appendix B to 10CFR50. In particular, the vent system shall be designed to ensure a low probability that (A) the vents will not perform their safety functions and (B) there would be inadvertent or irreversible actuation of a vent. Furthermore, the use of these vents during and following an accident must not aggravate the challenge to the containment or the course of the accident.

STATUS OF COMPLIANCE

Appropriate high point vents are provided at Millstone Unit No. 1 as identified in Attachment No. 3.

SECTION

50.44(d)(1)

REQUIREMENTS

For facilities that are in compliance with 10CFR50.46(b), the amount of hydrogen contributed by core metal-water reaction (percentage of fuel cladding that reacts with water), as a result of degradation, but not total failure, of emergency core cooling functioning shall be assumed either to be five times the total amount of hydrogen calculated in demonstrating compliance with 10CFR50.46(b)(3), or to be the amount that would result from reaction of all the metal in the outside surfaces of the cladding cylinders surrounding the fuel (excluding the cladding surrounding the plenum volume) to a depth of 0.00023 inch (0.0058mm), whichever amount is greater. A time period of 2 minutes shall be used as the interval after the postulated LOCA over which the metal-water reaction occurs.

STATUS OF COMPLIANCE

The extent of metal-water reaction calculated in demonstrating compliance with 10CFR50.46 is 0.19%. Five (5) times this value is approx-imately 1%. Our evaluation addresses metal-water reactions up to and beyond 1%.

SECTION

50.44(d)(2)

REQUIREMENT

For facitlities as to which no evaluation of compliance in accordance with 10CFR50.46(b) has been submitted and evaluated, the amount of hydrogen so contributed shall be assumed to be that amount resulting from the reaction of 5 percent of the mass of metal in the cladding cylinders surrounding the fuel, excluding the cladding surrounding the plenum volume.

STATUS OF COMPLIANCE

See Section 10CFR50.44(d)(1) above.

SECTION

50.44(e)

REQUIREMENT

For facilities whose notice of hearing on the application for a construction permit was published on or after November 5, 1970, purging and/or repressurization shall not be the primary means for controlling combustible gases following a LOCA. However, the capability for controlled purging shall be provided. For these facilities, the primary means for controlling combustible gases following a LOCA shall consist of a combustible gas control system, such as recombiners, that does not result in a significant release from containment.

STATUS OF COMPLIANCE

This is not applicable since Millstone Unit No. 1 received its construction permit (CPPR-20) on May 19, 1966.

SECTION

50.44(f)

REQUIREMENT

For facilities with respect to which the notice of hearing on the application for a construction permit was published between December 22, 1968, and November 5, 1970, if the incremental radiation dose from purging (and repressurization if a repressurization system is provided) occurring at all points beyond the exclusion area boundary after a postulated LOCA calculated in accordance with 10CFR100.11(a)(2) is less than 2.5 rem to the whole body and less than 30 rem to the thyroid, and if the combined radiation dose at the low population zone outer boundary from purging and the postulated LOCA calculated in accordance with 10CFR100.11(a)(2) is less than 25 rem to the whole body and less than 300 rem to the thyroid, only a purging system is necessary, provided that the purging system and any filtration system associated with it are designed to conform with the general requirements of Criteria 41, 42, and 43 of

Appendix A to 10CFR50. Otherwise the facility shall be provided with another type of combustible gas control system (a repressurization system is acceptable) designed to conform with the general requirements of Criteria 41, 42, and 43 of Appendix A to 10CFR50. If a purge system is used as part of the repressurization system, the purge system shall be designed to conform with the general requirements of Criteria 41, 42 and 43 of Appendix A to 10CFR50. The containment shall not be repressurized beyond 50 percent of the containment design pressure.

STATUS OF COMPLIANCE

This is not applicable since Millstone Unit No. 1 received its construction permit (CPPR-20) on May 19, 1966.

SECTION

50.44(g)

REQUIREMENT

For facilities with respect to which the notice of hearing on the application for a construction permit was published on or before December 22, 1968, if the combined radiation dose at the low population zone outer boundary from purging (and repressurization if a repressurization system is provided) and the postulated LOCA calculated in accordance with 10CFR 100.11 (a)(2) is less than 25 rem to the whole body and less than 300 rem to the thyroid, only a purging system is necessary, provided that the purging system and any filtration system associated with it are designed to conform with the general requirements of Criteria 41, 42, and 43 of Appendix A to 10CFR50. Otherwise, the facility shall be provided with another type of combustible gas control system (a repressurization system is acceptable) designed to conform with the general requirements of Criteria 41, 42, and 43 of Appendix A to 10CFR50. If a purge system is used as part of the repressurization system, it shall be designed to conform with the general requirements of Criteria 41, 42 and 43 of Appendix A to 10CFR50. The containment shall not be repressurized beyond 50 percent of the containment design pressure.

STATUS OF COMPLIANCE:

We interpret this section to require either a purging system designed to conform with General Design Criteria (GDC) 41, 42 and 43 or another type of combustible gas control system designed to conform with GDC 41, 42 and 43. The following illustrates our compliance with the latter. 10CFR50.44 (h)(2) defines a combustible gas control system as a system that operates after a LOCA to maintain the concentrations of combustible gases within the containment below flammability limits. By definition, to operate means to function effectively or to bring about a desired effect. Based on our evaluation, the inerted containment at Millstone Unit No. 1 functions quite effectively after a LOCA to maintain the concentrations of combustible gases within the containment below flammability limits. An inerted containment, which is a passive combustible gas control system, is in general conformance with GDC 41, 42 and 43.

SECTION

50.44(h)

REQUIREMENT

(h) As used in this section: (1) Degradation, but not total failure, of emergency core cooling functioning means that the performance of the emergency core cooling system is postulated, for purposes of design of the combustible gas control system, not to meet the acceptance criteria in 10CFR50.46 and that there could be localized clad melting and metal-water reaction to the extent postulated in 10CFR50.44(d). The degree of performance degradation is not postulated to be sufficient to cause core meltdown.

(2) A combustible gas control system is a system that operates after a LOCA to maintain the concentrations of combustible gases within the containment, such as hydrogen, below flammability limits. Combustible gas control systems are of two types: (i) Systems that allow controlled release from containment, through filters if necessary, such as purging systems and repressurization systems, and (ii) systems that do not result in a significant release from containment such as recombiners.

(3) A purging system is a system for the controlled release of the containment atmosphere to the environment through filters if needed.

(4) A repressurization system is a system used to dilute the concentration of combustible gas within containment by adding inert gas or air to the containment. Dilution of the combustible gas results in a delay in time until a flammable concentration is reached and permits fission product decay. Operation is limited to a containment repressurization to 50 percent of the containment design pressure. A purging system is normally part of the repressurization system.

STATUS OF COMPLIANCE

No specific requirements are contained in this section.

Docket No. 50-245

ATTACHMENT NO. 3

MILLSTONE NUCLEAR POWER STATION, UNIT NO. 1

COMBUSTIBLE GAS CONTROL EVALUATION

AUGUST, 1982

NORTHEAST UTILITIES

THE CONNECTICUT LIGHT AND POWER COMPANY
THE HARTFORD ELECTRIC LIGHT COMPANY
WESTERN MASSACHUSETTS ELECTRIC COMPANY
HOLYOKE WATER POWER COMPANY
NORTHEAST UTILITIES SERVICE COMPANY
NORTHEAST NUCLEAR ENERGY COMPANY

General Offices ● Selden Street, Berlin, Connecticut

P.O. BOX 270
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MAY 24, 1982
DOCKET NO. 50-245
A02389

Director of Nuclear Reactor Regulation
Attn: Mr. Dennis M. Crutchfield, Chief
Operating Reactors Branch #5
U. S. Nuclear Regulatory Commission
Washington, D.C. 20555

References:
(1) D. M. Crutchfield letter to W. G. Counsil, dated March 25, 1982.
(2) W. G. Counsil letter to D. G. Eisenhut, dated October 18, 1979.
(3) W. G. Counsil letter to H. R. Denton, dated November 21, 1979.
(4) W. G. Counsil letter to D. G. Eisenhut, dated August 20, 1981.
(5) W. G. Counsil letter to D. G. Eisenhut, dated December 31, 1981.
(6) T. D. Keenan letter to D. G. Eisenhut, dated October 17, 1979.
(7) D. L. Ziemann letter to W. G. Counsil, dated April 18, 1980.
(8) W. G. Counsil letter to D. M. Crutchfield, dated September 9, 1980.

Gentlemen:

MILLSTONE NUCLEAR POWER STATION, UNIT NO. 1
TMI ACTION ITEM II.B.1
REACTOR COOLANT SYSTEM VENTS

In Reference (1), Northeast Nuclear Energy Company (NNECO) was requested to provide additional information regarding reactor coolant system high point vents at Millstone Unit No. 1. Information was previously provided to the NRC Staff on this subject in References (2), (3), (4) and

(5). In these references, we indicated that we supported the position of the BWR Owners' Group (Reference (6)). Specifically we stated that sufficient inherent venting capability already exists at Millstone Unit No. 1 in the form of safety/relief valves (S/RV's), normally closed vessel head vent valves and a normally open vessel head vent line to the main steam line.

In response to a verbal request, we informed the NRC Staff in April 1980 that the tube side of the isolation condenser can be vented to the downstream side of the outside main steam line isolation valves through remote manual block valves. Based upon this information and that information provided to the NRC Staff in References (2) and (3), the NRC Staff indicated in Reference (7) that the TMI Category A requirements for this item have been satisfied.

10CFR50.44(c)(3)(iii), which became effective on January 4, 1982 and which codifies NRC requirements on reactor coolant system vents, requires that each light-water nuclear power reactor be provided with high point vents for the reactor coolant system, the reactor vessel head and other systems required to maintain adequate core cooling following a design basis loss-of-coolant accident (LOCA), if the accumulation of non-condensible gases would cause the loss of function of these systems.

Subsequent to receipt of Reference (1) and in light of 10CFR50.44(c)(3)(iii), the need to vent the isolation condenser was evaluated further. The results of the re-analysis of both the design basis and small-break LOCA are contained in Attachment No 2, "Loss of Coolant Accident Analysis Report for Millstone Unit 1 Nuclear Power Station," NEDO-24085-1, July 1980, to Reference (8). The operation of the isolation condenser is only credited in the small-break LOCA analysis and is, therefore, not required to maintain adequate core cooling following a design basis LOCA. Regarding a small-break LOCA and an assumed gas turbine failure, the function of the isolation condenser is to enhance depressurization prior to the actuation of the Automatic Depressurization System(ADS), which occurs in approximately 150 seconds. In this time interval, the peak cladding temperature would only be approximately 700°F and hydrogen generation from a metal-water reaction as well as radiolysis, would not yet be of concern. Pursuant to 10CFR50.44(c)(3)(iii), high point vents on the isolation condenser are not required since accumulation of non-condensible gases will not cause the loss of function of the isolation condenser during the very short period of time its operation is required. Therefore, responses to the various parts of Question No. 2 in Reference (1) are not necessary.

Extensive efforts are currently underway to accurately model the generation of hydrogen and oxygen following a LOCA at Millstone Unit No. 1. We intend to use the results of these efforts to evaluate whether modifications to the isolation condenser vent system would be desirable to allow the operation of the isolation condenser following an accident beyond the design basis of the plant.

In response to Question No. 1 in Reference (1), we have determined that there are no other systems required to maintain adequate core cooling where an accumulation of noncondensible gases could occur causing the loss of function of those systems. In arriving at this conclusion, the potential impact of non-condensible gases upon continued operation of the Feedwater Coolant Injection (FWCI), Low Pressure Coolant Injection (LPCI) and Core Spray (CS) Systems was assessed.

For the particular case of the FWCI System, which takes suction from the main condenser or condensate storage tank, the non-condensibles within the reactor coolant system will not affect its continued operation.

Venting of non-condensible gases from the reactor coolant system through the ADS valves will result in the accumulation of these gases in the torus. The potential for these gases to be dissolved in the torus water and to affect the operation of the LPCI and CS Systems, which take suction directly from the torus, was investigated. Even under design basis accident conditions, the torus temperature and pressure are not judged to be sufficient to dissolve significant quantities of non-condensible gases in the torus water. Further verification of this will be obtained when our ongoing efforts regarding hydrogen and oxygen generation following a LOCA are completed. Therefore, the accumulation of non-condensible gases will not occur such to cause a loss of function of either the LPCI or CS system. Additionally, the available net positive suction head, even under highly degraded conditions, is sufficient to ensure proper operation of the LPCI and CS pumps.

We trust that this response adequately responds to the NRC Staff's concerns raised in Reference (1).

Very truly yours,

NORTHEAST NUCLEAR ENERGY COMPANY

W. G. Counsil

W. G. Counsil
Senior Vice President

Docket No. 50-245

ATTACHMENT NO. 4

MILLSTONE NUCLEAR POWER STATION, UNIT NO. 1

COMBUSTIBLE GAS CONTROL EVALUATION

AUGUST, 1982

Analysis of Post-Accident Combustible Gas Control at Millstone Unit I

Volume I

Main Report

NOTICE

This report was prepared by Northeast Utilities Service Company (NUSCO) pursuant to a contract with Northeast Nuclear Energy Company (NNECO). Neither NUSCO nor NNECO, nor their employees, nor any other person acting on behalf of those companies makes any warranty or representation, express or implied, with respect to the use of any information, apparatus, product or process disclosed in this report with respect to its accuracy, completeness, or usefulness or that its use would not infringe privately owned rights, nor do the companies nor their employees, nor any other person acting on behalf of the companies assume any legal liability or responsibility with respect to the use of, or for damages which might result from the use of, any information, apparatus, product or process disclosed in this report.

ACKNOWLEDGEMENTS

NUSCo acknowledges the substantial comments and suggestions of the Radiation Chemistry Department of the AERE/Harwell Laboratory, U.K., who provided numerous insights in the development of the FACSIMILE post-accident radiolysis and recombination simulation model.

Additionally, the criticisms and suggestions of the Chemistry Division of Argonne National Laboratory were invaluable during the peer review process of this report.

The support of the B.W.R. Owner's Group is also ackowledged.

Northeast Utilities Service Company

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ABSTRACT

In response to the December 2, 1981 final rule on "Interim Requirements Related to Hydrogen Control," NUSCO on behalf of NNECO has conducted an engineering evaluation of hydrogen generation scenarios at the Millstone Unit 1 Boiling Water Reactor. The purpose of this evaluation was to determine quantitatively the existing level of hydrogen flammability control and to determine the incremental benefit (if any) of backfitting internal or external hydrogen recombiners. Assuming the Millstone Unit 1 (Mark I) containment is initially inerted with excess N_2 gas, (and, hence, O_2 content is at or below the 4% volume concentration) the following results have been obtained:

a. Preinerting with excess N_2 is so effective that H_2 generation (via $Zr-H_2O$ reactions) alone cannot yield flammable mixtures unless an additional source of oxygen is provided.

b. With removal of oxygen in-leakage from the M.S.I.V. and S/R valve control air lines, radiolysis is the only credible oxygen source present in the post-accident containment environment which could be dealt with via use of recombiners.

c. Radiolytic production of oxygen is in actuality limited to values substantially below those predicted in NRC Regulatory Guide 1.7 due to the fact that boiling within the core region ceases in a relatively short time and liquid phase recombination in a radiation field is significant.

Preinerting of the containment is thus sufficient by itself to prevent hydrogen combustion. Hence, there is no need for either recombiners, post-accident purging or post-accident N_2 addition.

CHAPTER 1

INTRODUCTION AND SUMMARY

1.0 INTRODUCTION

It is well recognized that the capability to control post-accident combustible gases is a critical safety function which must be present in order to assure containment integrity and long term decay heat removal. The assurance of post-accident combustible gas control capability is most critical for Mark I containment Boiling Water Reactors (B.W.R.s) due to their relatively small internal contaiment volumes and amount of zircaloy which could potentially become oxidized.

1.1 <u>THE COMBUSTIBLE GAS CONTROL RULE</u>

The accident at Three Mile Island Unit 2 produced extensive oxidation of the zircaloy cladding, and thus a large volume of hydrogen gas. The fuel cladding failure also resulted in the release of an appreciable quantity of airborne fission products within the containment. It was evident that venting as a means of hydrogen control in the event of extensive fuel failure and resultant airborne contamination would force an unwanted release of radioactivity to the environment.

With this perspective in mind, the NRC promulgated additional requirements (10-CFR-50.44) for post-accident combustible gas control in December 1981. These additional requirements mandated inerting for all Mark I containment B.W.R.s. Also required was the installation of internal $H_2 - O_2$ recombiners (or the capability to install external $H_2 - O_2$ recombiners immediately after a hypothetical accident) <u>for any reactor that relied on a purge/pressurization based system as the primary means for controlling combustible gases following a LOCA</u>.

NUSCO's assessment of this rule as it applies to the Millstone Unit I B.W.R. (Mark I Containment) considered the effectiveness of the N_2 inerting. Ultimately, it is shown that purge/pressurization is unnecessary <u>at any time</u> for combustible gas control.

1.2 CONTENTS OF THIS ANALYSIS

The analyses carried out in this report documents the following:

(i) the pre-accident initial gas concentrations for an inerted containment and their relationship to the limits of flammability. (This material is discussed in Chapter 2).

(ii) the short term generation of both hydrogen and oxygen as a result of zircaloy oxidation and boiling phase radiolysis - and how these processes alter H_2, O_2, and N_2 concentrations relative to the flammability limits. (This material is discussed in Chapter 3).

(iii) the long term radiolysis and recombination offsets in pure (and contaminated) water at different temperatures, flowing through the core at various volumetric flow rates, with different postulated initial H_2 and O_2 concentrations, - and how these processes either stabilize or reduce the initial H_2 and O_2 concentrations. (This material is discussed in Chapter 4).

1.3 SUMMARY OF SIGNIFICANT FINDINGS

The key results of this analysis may be summarized as follows:

(i) The most limiting combustible gas mixtures in the post-accident containment environment occur shortly after the time boiling ceases in the core. Following this time period, a net recombination of H_2 and O_2 is predicted to varying extents due to the natural tendency of excess dissolved H_2 and O_2 gas to recombine in the mixed β, γ radiation field of the reactor core.

(ii) The recombination rates are sensitive to the postulated volumetric core flow rates and water temperatures. (Higher flow rates and elevated water temperatures tend to promote a faster net recombination).

(iii) The impact of chemical and fission product impurities on blocking the natural recombination of H_2 and O_2 (via scavenging of H and OH radicals) is shown to be insufficient. This is true even when fission product contamination approaches the levels observed at TMI-2, and when metallic corrosion product impurities are assumed that are substantially higher than normally observed in B.W.R.s.

(iv) Inerting of the containment (with initial O_2 at 4% or less) is sufficient in itself to preclude flammable containment gas mixtures for an indefinite period without need for either purge/pressurization, or H_2 - O_2 recombiners.

CHAPTER 2

DEFINITION OF FLAMMABILITY LIMITS AND INITIAL (PRE-ACCIDENT) GAS CONCENTRATIONS

2.0 INTRODUCTION

In this section, the flammability limits utilized in the analysis are defined. A flammability criteria based on a numerical curvefit of the Coward-Jones flammability limits is presented along with data defining the levels of conservatism present in this curvefit.

Additionally, the initial conditions on gas concentrations at the start of an accident are defined and are related to the flammability limits. This is done in order to define the existing safety margin against flammability initially provided by containment inerting.

2.1 FLAMMABILITY LIMIT METHODOLOGY

In order to assess a wide range of scenarios where flammable gas mixtures are developed within the containment, it is first necessary to define what concentrations are needed to enter the flammable mixture regime. Published values obtained by Coward and Jones and reported in U.S. Bureau of Mines Bulletin No. 503 (Reference 1) are utilized in this evaluation. This data is in terms of ternary mixtures of H_2, O_2, and N_2. No data is presented for the additional effect of steam which is known to reduce the flammability potential. Concentrations referred to in this report are in terms of noncondensible gases and are defined as follows:

$$[H_2]_c = \frac{n_{H_2}}{n_{H_2} + n_{O_2} + n_{N_2} + n_x} \qquad (2.1a)$$

$$[O_2]_c = \frac{n_{O_2}}{n_{H_2} + n_{O_2} + n_{N_2} + n_x} \qquad (2.1b)$$

$$[N_2]_c = \frac{n_{N_2}}{n_{H_2} + n_{O_2} + n_{N_2} + n_x} \qquad (2.1c)$$

-where $[Gas]_c$ is the concentration relative to other noncondensible gases H_2, O_2, N_2, X found in the containment, n_{gas} is the number of moles of gas, "X" subscript refers to all other noncondensible gases found in the containment (e.g., CO_2, Ar, etc.).

It is important to recognize the fact that the number of moles of steam (n_{H_2O}) is not included in any calculations used in this report. This was done for three reasons:

1. The presence of steam reduces flammability potential; hence, its omission represents a significant conservatism in the results of this analysis.

2. The specific amount of steam released in an accident is highly scenario dependent ranging from a major pipe rupture to various types of loss of feedwater events with an intact RCS. Eliminating the n_{H_2O} dependence provides a conservative analysis which bounds the widest possible spectrum of accident scenarios.

3. The accident scenarios evaluated in this report have the common characteristic that steam is generated (during certain time periods) within the core in the drywell volume and condensed within the torus suppression pool. The addition of steam in one volume and its removal in another gives an appearance of nonuniformity of H_2 content among the two volumes; hence, elimination of steam allows one to conservatively concentrate on the critical H_2 and O_2 concentrations.

Having eliminated the steam concentration effects, the noncondensible gases may be conservatively treated as uniformly distributed between the drywell and torus volumes. Mixing of the gases between the drywell and torus volumes is assured and is documented in Reference 11.

To facilitate numerical calculations, the existing flammability limit data (Reference 1) was numerically fitted using a standard IBM-370 curvefitting package (Reference 2). The resultant curvefit is shown in Figure 1. The upper region curve is defined (within the region of interest) by the following equation:

$$[H_2]_{lim} = \sum_{m=0}^{3} A_m [O_2]_c^m \qquad (2.2)$$

where:

$A_o = -0.7119376 \times 10^2$

$A_1 = 0.2020868 \times 10^2$

$A_2 = -0.10543 \times 10^1$

$A_3 = 0.1990303 \times 10^{-1}$

Using this curvefit, flammability is conservatively assumed whenever:

$$0.04 \leq [H_2]_c \leq [H_2]_{lim} \qquad (2.3)$$

- for a given value of $[O_2]_c$ in the range $0.05 \leq [O_2]_c \leq 0.17$

The computer run and error analysis for this curve fit are found in the Appendix A in Volume II.

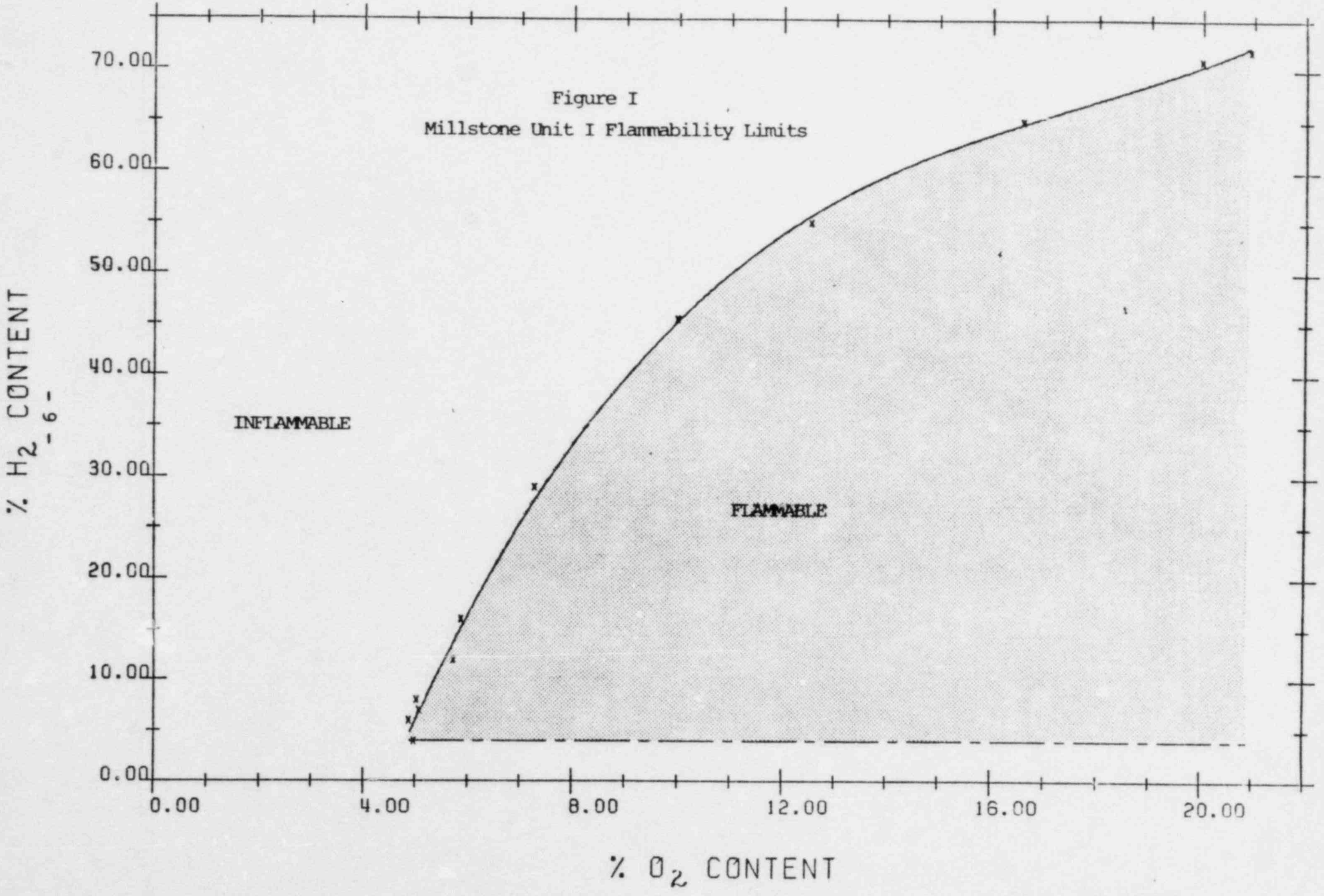

Figure I

Millstone Unit I Flammability Limits

MILLSTONE 1 FLAMMABILITY LIMITS

As an additional note on the conservatism employed in using these flammability limits, it should be pointed out that hydrogen and oxygen concentrations just inside the flammability limits were determined in vessels and vertical pipes with a spark igniter provided as an ignition source. Spontaneous ignition of hydrogen and oxygen mixtures requires significantly higher concentrations (e.g., 18% H_2 in air). Furthermore, actual experimental tests (References 3 and 4) indicate the existence of unstable flames and an incomplete combustion process for hydrogen concentrations in normal air less than 8%. Due to the unstable flames and incomplete combustion processes, the actually observed pressure rises are substantially below the theoretical pressure rise values calculated assuming a complete adiabatic burn (e.g., 1 psi versus calculated values in the range of 23-40 psi). Hence, approach to the flammability limit lines does not pose any imminent threat to containment integrity as a result of hydrogen burns. In view of this, the flammability limits defined above may be used directly as a conservatively biased acceptance level.

2.2 INITIAL CONTAINMENT GAS COMPOSITION

Having defined the limits of flammability, it is now necessary to identify the initial starting points for sequences where flammability is approached. Normal (noninerted) air contains the following concentrations of gases:

(Reference 3)

H_2	0.00005%
N_2	78.084%

O_2	20.946%	
CO_2	0.033%	"X"
Ar	0.943%	

Under inerted conditions, these concentrations are substantially different.

- o While under normal operations, the containment gas composition is required by Technical Specification 3.7.A.6 to maintain an O_2 content of less than 5%. Procedurally, however, in order to avoid violation of plant technical specifications, additional N_2 is added to assure O_2 never actually exceeds 4%.

- o Based on operating experience at other plants, it has been observed that small amounts of H_2 (above normal atmospheric concentrations) can be found in containment. This is postulated to be a result of nominal long-term H_2 leakage from the steam lines through the M.S.I.V.s and S/R valves. It is conservatively[*] estimated that this may amount to as much as 0.1%.

- o Nitrogen (N_2) and other inert gases will comprise the remainder.

---

[*] Inclusion of this small amount of additional hydrogen is a conservatism in that it reduces the amount of net radiolysis needed to reach flammability when a very small metal-water reaction has occurred.

In order to calculate initial and post-accident containment gas concentrations, it is noted that Millstone Unit 1 has the following free air volumes.

Drywell: $146,900\ \text{ft}^3$
Torus*: $108,200\ \text{ft}^3$ (Minimum)
$110,600\ \text{ft}^3$ (Maximum)

The number of liters of gas contained within the drywell can be obtained by multiplication of the volume in ft^3 by the conversion factor 28.316 liters/ft^3. As an additional factor of conservatism, the smaller torus gas volume is used yielding

$$V_{\text{containment}} = 7.291 \times 10^6 \text{ liters} \qquad (2.4)$$

The total number of moles of gas initially present in the containment may be conservatively, determined via the Ideal Gas Law assuming an initial pressure of 1.0 atmosphere and a temperature of 325°K. **

$$n_{\text{gas}} = \frac{p\ V_{\text{containment}}}{RT} = 2.7085 \times 10^5 \text{ moles} \qquad (2.5)$$

---

*The gas space volume in the Torus Region is water level dependent. Technical specification limits exist for allowable water level.

** If conservatively biased EEQ temperature and two region pressure values were utilized, 4% more initial gas would be available to dilute any generated gases.

Using the previously defined initial concentrations, the corresponding numbers of moles of the various gases will be:

$$n_{H_2} = 2.7 \times 10^2 \text{ moles (or .1\%)} \qquad (2.6a)$$

$$n_{O_2} = 1.08 \times 104 \text{ moles (or 4\%)} \qquad (2.6b)$$

$$n_{N_2} + n_x = 2.6 \times 10^5 \text{ moles (or 95.9\%)} \qquad (2.6c)$$

2.3 INITIAL GASES DISSOLVED IN THE TORUS WATER

In addition to gases in the free air volumes, gases will also be dissolved in the torus water up to the equilibrium limits of solubility for the gas in question. Hence, the gas partial pressures in the containment atmosphere represent an equilibrium effect. The extent of these gases in solution may be calculated based on Henry's Law. Assuming a net torus pressure of approximately 1.0 atmosphere, the following mole fractions will exist.

$$\frac{n_{H_2}}{n_{H_2} + n_{O_2} + n_{N_2} + n_x} = 0.001 \tag{2.7a}$$

$$\frac{n_{O_2}}{n_{H_2} + n_{O_2} + n_{N_2} + n_x} = 0.04 \tag{2.7b}$$

$$\frac{n_{N_2}}{n_{H_2} + n_{O_2} + n_{N_2} + n_x} \cong 0.959 \tag{2.7c}$$

These values would correspond to the following gas partial pressures:

$$p_{H_2} = .0147 \text{ psi} \tag{2.8a}$$

$$p_{O_2} = .588 \text{ psi} \tag{2.8b}$$

$$p_{N_2} = 13.097 \text{ psi} \tag{2.8c}$$

(assumes: $N_2 + X \cong N_2$)

The solubilities based on Henry's Law may be defined:

$$S_i\left(\frac{\text{cm}^3\ \text{gas}}{\text{k}_g\ \text{H}_2\text{O}}\right) = \frac{8.45 \times 10^4\ \text{Pi}}{H_i} \tag{2.9}$$

- where S_i is the solubility in units of cm^3 of dissolved gas per kg of H_2O, p_i is the partial pressure in psi, and H_i is the Henry's Law constant for the temperature region of interest.

For the temperature region of interest ($T \leq 90°F$) the Henry constants (Reference 5) are respectively:

$$H_{H_2} = 7.46 \times 10^4$$

$$H_{O_2} = 5.24 \times 10^4$$

$$H_{N_2} = 10.26 \times 10^4$$

Use of these values yields the following solubilities which are converted to molar concentration by multiplying by 4.46428×10^{-5} moles/cm^3:

$$S_{H_2} = 1.665 \times 10^{-2}\ \frac{\text{cm}^3\ \text{H}_2}{\text{k}_g\ \text{H}_2\text{O}} = 7.433 \times 10^{-7}\ \text{moles/liter} \tag{2.10a}$$

$$S_{O_2} = 9.482 \times 10^{-1}\ \frac{\text{cm}^3\ \text{O}_2}{\text{k}_g\ \text{H}_2\text{O}} = 4.233 \times 10^{-5}\ \text{moles/liter} \tag{2.10b}$$

$$S_{N_2} = 1.161 \times 10^{-1}\ \frac{\text{cm}^3\ \text{N}_2}{\text{k}_g\ \text{H}_2\text{O}} = 5.183 \times 10^{-4}\ \text{moles/liter} \tag{2.10c}$$

There is a total* of roughly 9.2×10^4 ft^3 (2.605×10^6 liters) of water in the torus; hence, the total number of moles of dissolved gases in liquid would be as follows:

$$(n_{H_2})_{liq} = S_{H_2} V_{liq} = 1.936 \times 10^{0} \text{ moles } H_2 \qquad (2.11a)$$

$$(n_{O_2})_{liq} = S_{O_2} V_{liq} = 1.103 \times 10^{2} \text{ moles } O_2 \qquad (2.11b)$$

$$(n_{N_2})_{liq} = S_{N_2} V_{liq} = 1.35 \times 10^{3} \text{ moles } N_2 \qquad (2.11c)$$

Thus, we note that the amount of gas dissolved in the torus water is roughly a percent of the total gas within the containment volume.

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*This is a 6% conservatism due to the fact Tech Spec. 3.7.A.1 requires a torus inventory of 9.8×10^4 ft^3. This analyses consistly uses the smaller liquid inventory to minimize dilution effects of impurities.

CHAPTER 3

DEFINITION OF SHORT-TERM HYDROGEN AND OXYGEN SOURCE TERMS

3.0 INTRODUCTION

In Chapter 2, the initial conditions for containment gas concentration were defined and related to the limits of flammability. In Chapter 3, the effects of various accident scenarios on containment H_2 and O_2 concentrations are defined by parametrically separating the effects of the metal-water reaction from the radiolytic decomposition of coolant water. This can be done by noting the fact that a metal-water reaction is phenomenologically related to short-term (within the first hour) overheating of the reactor fuel due to insufficient core cooling, whereas radiolytic decomposition is due to long-term (over many hours) exposure of reactor coolant to radiation. Thus, as an analytical technique, the effects of the short-term metal-water reaction are treated first. For a given metal-water reaction, additional analysis is then performed to define the effects and extent of longer-term radiolytic decomposition. The critical parameter affecting radiolytic decomposition extent is shown to be the duration of boiling in the core. Short-term boiling is shown to result in containment gas concentrations which are substantially less than the flammability limits.

3.1 HYDROGEN GENERATION VIA METAL-WATER REACTION

When the reactor core is inadequately cooled (uncovered) for sustained periods of time, the zircaloy cladding in the fuel assemblies will begin to rapidly heat up, creating the potential for a high temperature Zr-H_2O reaction. Numerous models have been developed to define the reaction kinetics. The specific kinetics of the Zr-H_2O reaction are not as important as the net amount of Zr reacted. As this reaction proceeds, H_2 gas is generated according to the following chemical reaction:

$$Zr + 2H_2O \rightarrow ZrO_2 + 2H_2 + \Delta Q \qquad (3.1)$$

For this reaction, it is noted that for each mole of Zr reacted, two moles of H_2 gas are generated. Hence, the net number of moles of H_2 generated may be related to the fraction of the total Zr reacted. Thus:

$$\Delta n_{H_2} = 2f_{Zr-H_2O}\, n_{Zr} \qquad (3.2)$$

- where f_{Zr-H_2O} is the extent of the metal-water reaction and lies between 0.0 and 1.0.

Assuming only the Zr-H_2O reaction as a short-term H_2 source, the impact on the containment gas concentrations is defined by the following equations.

$$[H_2]_c = \frac{n_{H_2} + \Delta n_{H_2}}{n_{H_2} + \Delta n_{H_2} + n_{O_2} + n_{N_2} + n_x}$$

$$= \frac{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr}}{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr} + n_{O_2} + n_{N_2} + n_x} \qquad (3.3a)$$

$$[O_2]_c = \frac{n_{O_2}}{n_{H_2} + \Delta n_{H_2} + n_{O_2} + n_{N_2} + n_x}$$

$$= \frac{n_{O_2}}{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr} + n_{O} \, {}_{2}+ N_{N} \, {}_{2}+ n_x} \qquad (3.3b)$$

The total amount of Zr in the cladding may be obtained by noting: $V_{clad} = 2.45 \times 10^5$ in^3 (Reference 6). Assuming the zircaloy cladding is all Zr (actually zircaloy is 98.5% Zr, Reference 7).

$$n_{Zr} = \frac{M_{Zr}}{91.22 \text{ gr/mole Zr}} = \frac{V_{clad}\,\rho_{Zr}}{91.22 \text{ gr/mole Zr}} = 3.529 \times 10^5 \text{ moles Zr} \qquad (3.4)$$

Utilizing the initial values of containment gases derived in Section 2.2, Figure II was obtained by parametrically varying f_{Zr-H_2O} between 0.0 and 1.0. A simple computer program to obtain $[H_2]_c$ and $[O_2]_c$ is shown in Appendix B in Volume II.

A significant observation to be drawn from this curve (Figure II) is the fact that short-term metal-water reactions alone (which produce only H_2 gas) are insufficient to yield flammable gas mixtures in the containment. Furthermore, more extensive metal-water reactions yield states further away from the flammability limits.

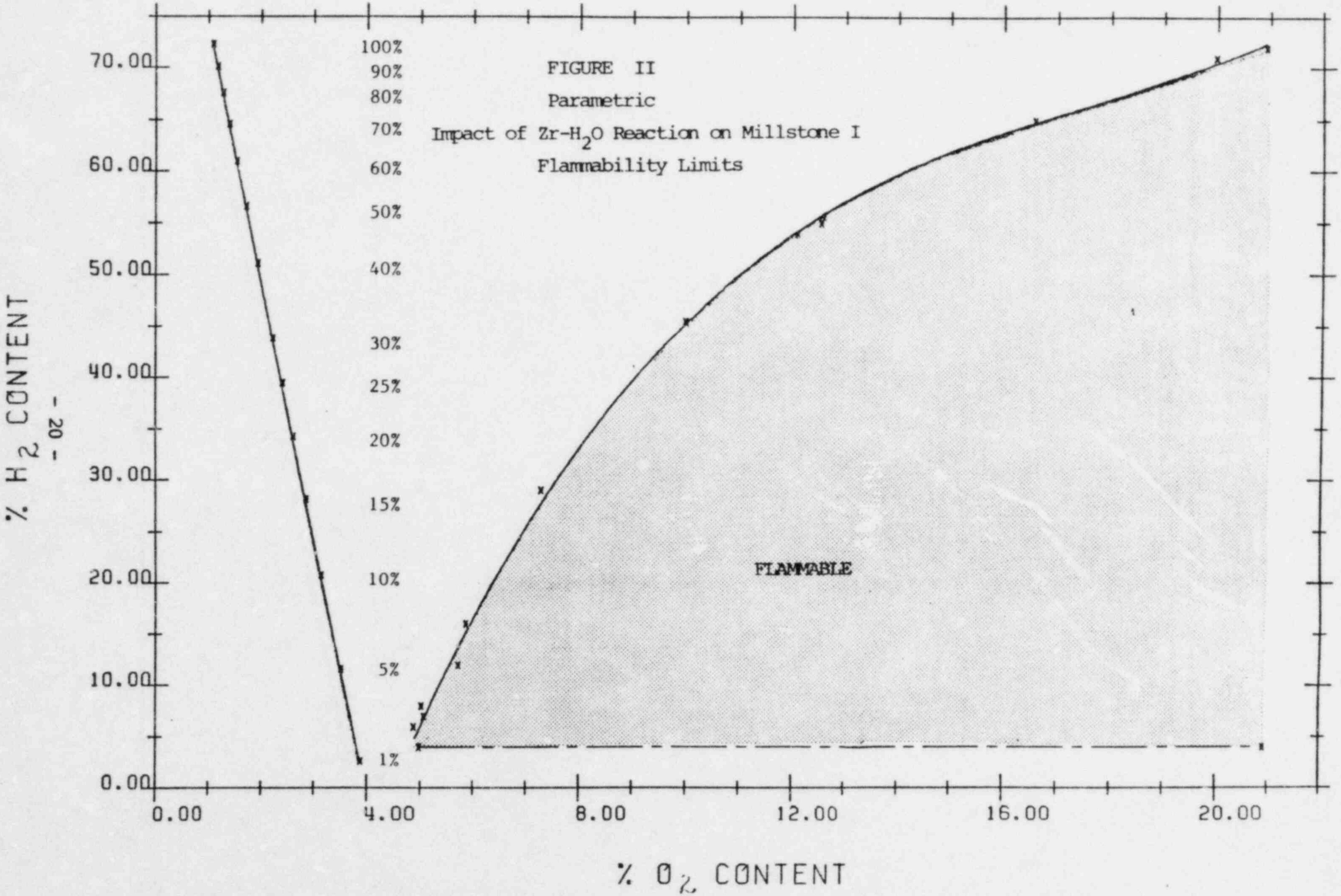

FIGURE II

Parametric

Impact of Zr-H_2O Reaction on Millstone I

Flammability Limits

MILLSTONE 1 FLAMMABILITY LIMITS

3.2 HYDROGEN AND OXYGEN GENERATION VIA RADIOLYSIS

Having independently assessed the effects on containment gases due to a short-term metal-water reaction, the effects of radiolytic decomposition of reactor coolant must be assessed. Should net radiolytic decomposition occur, it would proceed via the following net reaction.

$$2H_2O \xrightarrow{n,\ \beta,\ \gamma} 2H_2 + O_2 \qquad (3.5)$$

Utilizing the fact that decomposition of 1 lb. of H_2O yields respectively 25.178 moles of H_2 gas and 12.589 moles of O_2 gas, the net increase in the containment inventories of H_2 and O_2 may be expressed via the following relationships:

$$\Delta n_{H_2}' = \varepsilon_{H_2O} X_{H_2} \qquad X_{H_2} = \frac{25.178 \text{ moles } H_2}{\text{lb. } H_2O} \qquad (3.6a)$$

$$\Delta n_{O_2}' = \varepsilon_{H_2O} X_{O_2} \qquad X_{O_2} = \frac{12.589 \text{ moles } O_2}{\text{lb. } H_2O} \qquad (3.6b)$$

Where ε_{H_2O} is defined as the extent of H_2O decomposed by radiolysis, defined in lb. H_2O.

Using these relationships, the impacts of any net radiolysis on containment gases (in addition to the metal-water reaction) is given by the following equations:

$$[H_2]_c = \frac{n_{H_2} + \Delta n_{H_2} + \Delta n'_{H_2}}{n_{H_2} + \Delta n_{H_2} + \Delta n'_{H_2} + n_{O_2} + \Delta n'_{O_2} + n_{N_2} + n_x}$$

$$= \frac{n_{H_2} + 2f_{Zr\text{-}H_2O}\, n_{Zr} + \varepsilon_{H_2O}\, X_{H_2}}{n_{H_2} + 2f_{Zr\text{-}H_2O}\, n_{Zr} + \varepsilon_{H_2O}\,(X_{H_2} + X_{O_2}) + n_{O_2} + n_{N_2} + n_x} \qquad (3.7a)$$

$$[O_2]_c = \frac{n_{O_2} + \Delta n'_{O_2}}{n_{H_2} + \Delta n_{H_2} + \Delta n'_{H_2} + n_{O_2} + \Delta n'_{O_2} + n_{N_2} + n_x}$$

$$= \frac{n_{O_2} + \varepsilon_{H_2O}\, X_{O_2}}{n_{H_2} + 2f_{Zr\text{-}H_2O}\, n_{Zr} + \varepsilon_{H_2O}\,(X_{H_2} + X_{O_2}) + n_{O_2} + N_{N_2} + n_x} \qquad (3.7b)$$

In the formation of these equations, no attempt is made at present to assess the likelihood of achieving specific values of ε_{H_2O}. (This assesment is provided in Section 3.3.) The purpose is to define the required extent of radiolysis needed to yield flammable mixtures. Using these equations which are scenario dependent (e.g., dependent on the extent of metal-water reaction and extent of radiolysis), specific scenarios yielding gas concentrations which are flammable can now be identified. The specific scenarios leading to flammable mixtures were defined by first assuming a specific value of $f_{Zr\text{-}H_2O}$ and then varying ε_{H_2O} until the flammability limit defined by the curvefit (Equation 2.2) is reached.

To facilitate a large number of these calculations, a short computer program was written (see Appendix C in Volume II). Utilizing this code, the table in Figure III was generated. Figure III shows the flammability limiting values of ε_{H_2O} for a given f_{Zr-H_2O}. Figure IV is a graph of these values.

Based on these scenario calculations, it is noted the minimal value of ε_{H_2O} results from a transition from the initial conditions: $[H_2]_c$ = .001 and $[O_2]_c$ = .04 to the point $[H_2]_c$ = 0.04, $[O_2]_c$ = 0.05. The changes in the number of moles of H_2 and O_2 (Δn_{H_2}, $\Delta n'_{H_2}$, and $\Delta n'_{O_2}$, respectively) necessary to reach this limit are defined by the following simultaneous equations:

$$0.04 = \frac{n_{H_2} + \Delta n_{H_2} + \Delta n'_{H_2}}{n_{H_2} + \Delta n_{H_2} + \Delta n'_{H_2} + n_{O_2} + \Delta n'_{O_2} + n_{N_2} + n_x} \qquad (3.8a)$$

$$0.05 = \frac{n_{O_2} + \Delta n'_{O_2}}{n_{H_2} + \Delta n_{H_2} + \Delta n'_{H_2} + n_{O_2} + \Delta n'_{O_2} + n_{N_2} + n_x} \qquad (3.8b)$$

Inserting the initial values of n_O , n_H , n_N , n_x (from Section 2.2) and algebraically solving yields the following:

$$\Delta n_{H_2} + \Delta n'_{H_2} = 1.12 \times 10^4 \text{ moles } H_2 \qquad (3.9a)$$

$$\Delta n'_{O_2} = 3.44 \times 10^3 \text{ moles } O_2 \qquad (3.9b)$$

Making use of the fact that oxygen is only produced via radiolysis (along with hydrogen at the stoichiometric ratio), it may be concluded that production of 3.44×10^3 moles O_2 is the result of radiolytic decomposition of 6.88×10^3 moles of H_2O, which would weigh 273.25 lbs.

FIGURE III

RADIOLYTIC DECOMPOSITION NECESSARY TO ACHIEVE FLAMMABILITY FOR A SPECIFIC $Zr-H_2O$ REACTION

Extent of $Zr-H_2O$ Reaction f_{Zr-H_2O}	Extent of Radiolytic Decomposition of H_2O ε_{H_2O} (lbs.)
.0050	304
.0055	290
.0058	281
.0059	278
.0060	275
.007	276
.009	283
.01	286
.015	303
.02	369
.03	482
.04	600
.05	721
.06	845
.07	974
.08	1,106
.09	1,242
.10	1,381
.11	1,525
.12	1,673
.13	1,824
.14	1,980
.20	3,002
.30	5,082
.40	7,730
.50	11,067

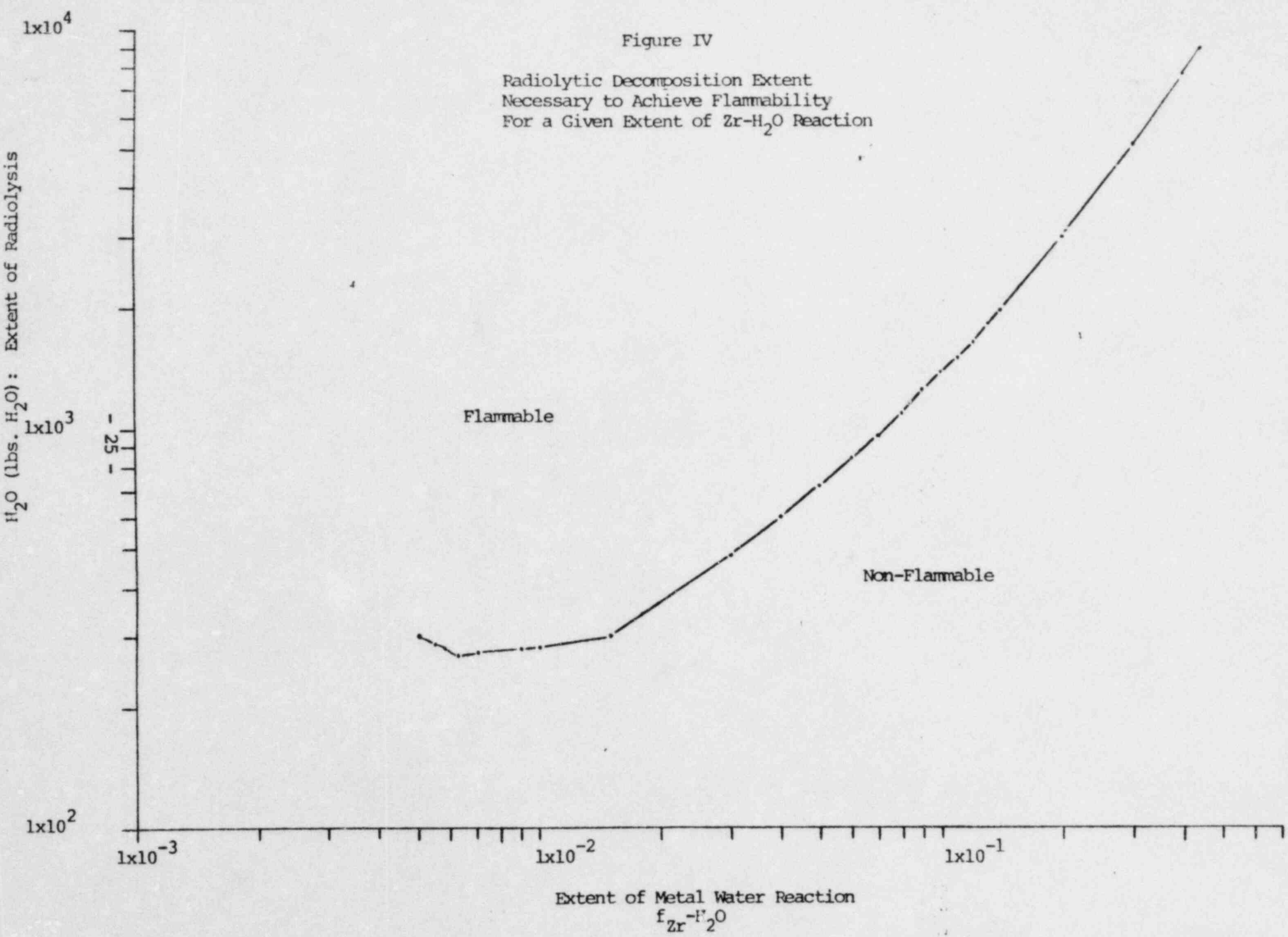

Figure IV

Radiolytic Decomposition Extent Necessary to Achieve Flammability For a Given Extent of Zr-H_2O Reaction

Additionally, the H_2 not produced by radiolysis would amount to 4.32×10^3 moles. This would correspond to a metal-water reaction extent of $f_{Zr-H_2O} = 0.00612$.

A number of significant observations may be drawn from the results of these scenario calculations:

- The most limiting range of metal-water reactions for the inerted Millstone I containments is for very small metal water reactions and not values in excess of 75% (Reference 8).
- The most limiting metal-water reaction is for $f_{Zr-H_2O} = 0.00612$. This requires radiolytic decomposition of only 273.25 lbs. of H_2O in order to reach potentially flammable conditions. All other metal-water reactions will require more radiolysis to yield flammable mixtures.
- Containment flammability for metal-water reactions in the range of $f_{Zr-H_2O} \leq 0.00612$ are limited by the lower limit line defined by $[H_2]_c = 0.04$ for $[O_2]_c \geq 0.05$ (i.e., they approach the flammable region from the bottom).
- Containment flammability for metal-water reactions in the range of $f_{Zr-H_2O} > 0.00612$ are limited by the upper flammability curve which varies as a function of $[O_2]_c$ (i.e., these sequences approach the flammable region from the side).

3.3 ASSESSMENT OF THE POTENTIAL FOR POST-ACCIDENT RADIOLYSIS

In Section 3.2, specific scenarios leading to potentially flammable gas mixtures were defined in terms of the parameters f_{Zr-H_2O} and ε_{H_2O}. It was noted at the time that a detailed evaluation was necessary to determine whether or not excessively large values of ε_{H_2O} were, in fact, credible. To properly perform a detailed evaluation of radiolysis, it is necessary to understand the basic physics involved in the process.

Net radiolytic decomposition of water into H_2 and O_2 occurs when water molecules interact with energetic α, β, γ, or neutrons. As a result of slowing down collisions, Compton electrons are generated, which have sufficient energy to break up the molecular bonds holding water molecules together. The net result is the generation of a series of free radicals, molecules, and aqueous electrons (e_{aq}^-, H, H_2, H_2O_2, OH, HO_2). Different radiation types are known to produce different yields of these species. The table in Figure V summarizes the known yields based on a compilation by Cohen in Reference 9.

Neutron effects are known to dominate during normal power operation and for the first several hundred seconds following reactor shutdown. Following normal reactor shutdown, the γ-dose would tend to become the dominant effect with a lesser contribution from β-particles (the majority of which are stopped by the fuel and cladding). Where fuel failures are postulated to exist, the effects of α and β-type radiations can become larger due to the presence of dissolved

	e^-	$H + e^-$	H	H_2	H_2O_2	OH	HO_2	AVERAGE L.E.T
mixed γ, β	2.31	2.86	0.55	0.44	0.70	2.34	0.00	.02 eV
γ	2.60	----	0.55	0.45	0.70	2.60	0.02	.02 eV
n	0.36	0.72	0.36	1.12	1.00	0.47	0.17	4.0 eV
$^{10}B(n, \gamma)^7Li$	0.04	0.20	0.16	1.70	1.30	0.10	0.30	24.0 eV

Initial Radiolytic Yields G_x in $\frac{\text{molecules}}{100\ \text{eV}}$

Figure V

fission products in the water. In view of the fact that the initial yields for α-particles is roughly four times the value for mixed β, γ radiations, and that α-particles are roughly 1,200 times more ionizing, one might expect the results for cases where extensive fuel damage has occurred to produce extensively more H_2 and O_2. Haissinsky, however, notes in Reference 9 that α-particles do not show significant differences in terms of net yields from those exhibited by γ-rays. The most likely explanation for this effect lies in the fact that because α-particles are so densely ionizing and, thus, leave such short ionization tracks (or "spurs"), the recombination effects are heavily affected by charged particles diffusing over very short distances.*

Following the initial production of the aqueous electrons, free radicals, and molecules, numerous chemical back reactions are possible. These reactions promote a recombination back to H_2O provided the radicals are allowed time and space to interact. It has generally been recognized that boiling systems disrupt this recombination due to the fact steam voids exist which prevent the diffusion processes. Boiling also causes the stripping of dissolved H_2 and O_2 gases from solution. The net effect is that appreciable quantities of H_2 and O_2 are liberated during boiling. This net production occurs at very near the stoichiometric ratio for H_2 and O_2.

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*Additionally in terms of net energy deposited in a unit of coolant volume the total β, γ dose is higher than the total α dose.

For nonboiling systems, recombination is enhanced to the level that essentially an equilibrium condition is found to exist between the net production and removal rates.

Because of the fact that all BWR accident scenarios inevitably involve a transition from a boiling phase to a nonboiling phase, post-accident radiolysis may be modelled as a two-step process. During the initial boiling phase, net decomposition of water occurs dependent only on radiation dose intensity and the net yields. As subcooling is achieved in the core and a nonboiling state is achieved, a radiochemical equilibrium is achieved defined by the reaction equation.

$$2H_2O \overset{\gamma,\beta}{\leftrightarrows} 2H_2 + O_2 \tag{3.10}$$

During this phase, equilibrium levels of H_2 and O_2 are achieved in both the coolant liquids and in the containment gases. Hence, what becomes significant is the determination of precisely how long boiling occurs.

As a part of the GE Owner's Group effort (Reference 11) on post-accident H_2 control, a detailed review was conducted of a number of accident scenarios to determine a maximum upper bound on the boiling time for design basis accidents. In this effort, boiling time was explicitly defined as the time period between reactor vessel isolation and attainment of a subcooled state in the reactor core. For large break LOCA's with full ECCS operation, it was assumed* that subcooling (and a cessation of boiling) could be expected within 130 minutes (~8 x 10^3 seconds). For the case of isolation transients and very small break LOCA scenarios involving only the use of low pressure ECCS (Core Sprays and Low Pressure Coolant Injection), a time period of up to 7.0 hours (2.52 x 10^4 seconds) would be required in order achieve subcooling. This seven hour bound includes a consideration of the scenarios involving operator actions to depressurize the vessel according to relevant emergency procedure guidelines.

For the purposes of analyzing radiolytic H_2 and O_2 production, a time period of 12 hours is assumed during which full core boiling is assumed to occur. After this time period, net subcooling within the core is assumed.

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* This assumption includes an additional 100-minutes for conservatism. Actual LOCA analyses indicate that approximately 30-minutes would in general be sufficient for a DBA LOCA for nominal injection flows.

3.3.1 RADIOLYTIC DECOMPOSITION DURING THE BOILING PHASE

During the boiling phase (post-accident), it is recognized that the net radiolytic yield of H_2 will conservatively approach the initial yields of H_2 from direct radiolysis (Reference 12). Oxygen (O_2) generation will conservatively proceed according to the stoichiometric ratio for decomposition of water. (This is very conservative in view of the fact that vapor phase recombination in the presence of γ-rays is appreciable. The impacts of vapor phase H_2 - O_2 recombination is discussed in Appendix D of Volume II.) Hence:

$$G(H_2) \cong G_{H_2} \qquad (3.11a)$$

$$G(O_2) = \tfrac{1}{2}\, G(H_2) \cong \tfrac{1}{2}\, G_{H_2} \qquad (3.11b)$$

The rate at which water is decomposed (in units of lbs./sec.) may be expressed as:

$$\dot{M}_{H_2O}(t) = \frac{2.2 \times 10^{-5}\, P_o\, E_{\beta,\gamma}(t)}{N_o}\left(G_{H_2}\, m_{H_2} + G_{O_2}\, m_{O_2}\right) \qquad (3.12)$$

- where:

P_o is the initial core thermal power, or 2,051 MW_t (corresponding to the 102% licensed power value)

N_o is Avogadro's number, $N_o = 6.023 \times 10^{23}$ molecules/mole

$E_{\beta, \gamma}(t)$ is the β, γ decay power as a function of time

m_{H_2} is the molecular weight of H_2, $m_{H_2} = 2.106$ grams/mole

m_{O_2} is the molecular weight of O_2, $m_{O_2} = 31.999$ grams/mole

The β, γ decay function defining the amount of energy absorbed by reactor coolant is similar to that specified in NRC Regulatory Guide 1.7 (References 13 and 14).

$$E_{\beta, \gamma}(t) = f_{\beta, \gamma} K_o \sum_i k_i e^{-\lambda_i t} \qquad (3.13)$$

- where:

$f_{\beta, \gamma}$ is the fraction of energy absorbed in the reactor coolant

$K_o = 1.0 \times 10^{22}$

The constants defining the decay energy curve are as follows:

$k_1 = 5.1912$	$\lambda_1 = 9.8 \times 10^{-5}$
$k_2 = 0.8743$	$\lambda_2 = 6.5 \times 10^{-6}$

$k_3 = 0.6557$ $\lambda_3 = 5.7 \times 10^{-7}$

$k_4 = 0.4098$ $\lambda_4 = 7.4 \times 10^{-8}$

$k_5 = 0.0150$ $\lambda_5 = 8.0 \times 10^{-10}$

By integrating $\dot{M}_{H_2O}$ (t), the net mass of water decomposed by radiolysis can be defined as a function of time and compared to the mass generated during the known boiling phase (e.g., ~ 8 x 10^3 to 4.32×10^4 seconds).

$$M_{H_2O} (t) = \int_o^t \dot{M}_{H_2O} (t') \, dt'$$

$$= A_o \, P_o \, f_{\beta,\gamma} \, (G_{H_2} \, m_{H_2} + G_{O_2} \, m_{O_2}) \sum_i \frac{ki}{\lambda i} (1-e^{-\lambda_i t}) \tag{3.14}$$

where: $A_o = 3.6526 \times 10^{-7}$

To facilitate a large number of sensitivity calculations based on this equation, a short computer program was written to evaluate H_2O decomposition vs. time. This program and sample outputs are discussed in Appendix E of Volume II. The range of parameters studied in the sensitivity calculations are shown in the table on Figure VI.

Two cases define the upper and lower limits of Radiolytic decomposition of H_2O during the boiling phase. An upper limit case is defined by using the 102% licensed power value (e.g., 2,051 MW_t), and setting: $f_{\beta,\gamma} = 0.094$, $G_{H_2} = 0.44$, $G_{O_2} =$

FIGURE VI

KEY PARAMETERS AFFECTING BOILING PHASE RADIOLYSIS

Parameter	Definition	Upper Bound	Lower Bound
P_o	Core Power Level	2,051 MW_t (102% value)	2,011 MW_t (100% value)
$f_{\beta, \gamma}$	Energy fraction absorbed in reactor coolant	0.094(1)	0.05(2)
G_{H_2}	Radiolytic H_2 yield	0.44(3)	0.20(4)
G_{O_2}	Radiolytic O_2 yield	0.22	0.10
T_B	Boiling Time	4.32×10^4	8×10^3

---

(1) Corresponds to the energy fraction absorbed in reactor coolant for coolant densities near the cold shutdown temperature.

(2) Corresponds to the energy fraction absorbed in reactor coolant for coolant densities in the temperature range of full power operation. The lower densities result in decreased energy absorption in the reactor coolant.

(3) Based on controlled laboratory measurements this value was used as an upper bound for G_{H_2} in lieu of the Reg. Guide 1.7 value of 0.50. (Reference 12).

(4) Based on experimental measurements and found to be conservative when compared to data from actual operating reactors (Reference 11).

0.22. The lower limit case is defined by using the nominal licensed power value (e.g., 2,011 MW_t) and setting: $f_{\beta, \gamma}$ = 0.094, G_{H_2} = 0.20, G_{O_2} = 0.10. Figure VII shows the results of these analyses including the time domain where boiling is assumed to cease.

Based on a review of the results of these analyses, the following conclusions may be drawn:

- The minimum amount radiolytic decomposition anticipated during the boiling phase is 14.0 lbs. This value is a result of assuming cessation of boiling at 30 minutes (1.8×10^3 sec.), nominal licensed power, and use of radiolytic yields of: G_{H_2} = 0.20 and G_{O_2} = 0.10.

- The maximum credible amount of radiolytic decomposition anticipated is 110.0 lbs. This value is a result of assuming persistent boiling (without any vapor phase recombination) until 12.0 hrs. (4.32×10^4 sec.), 102% licensed power, and use of radiolytic yields of: G_{H_2} = 0.44 and G_{O_2} = 0.22.

- The amount of radiolysis necessary to yield flammable conditions for the most limiting metal-water reaction is greater than 2.5 times the maximum credible amount of radiolytic decomposition anticipated during the boiling phase.

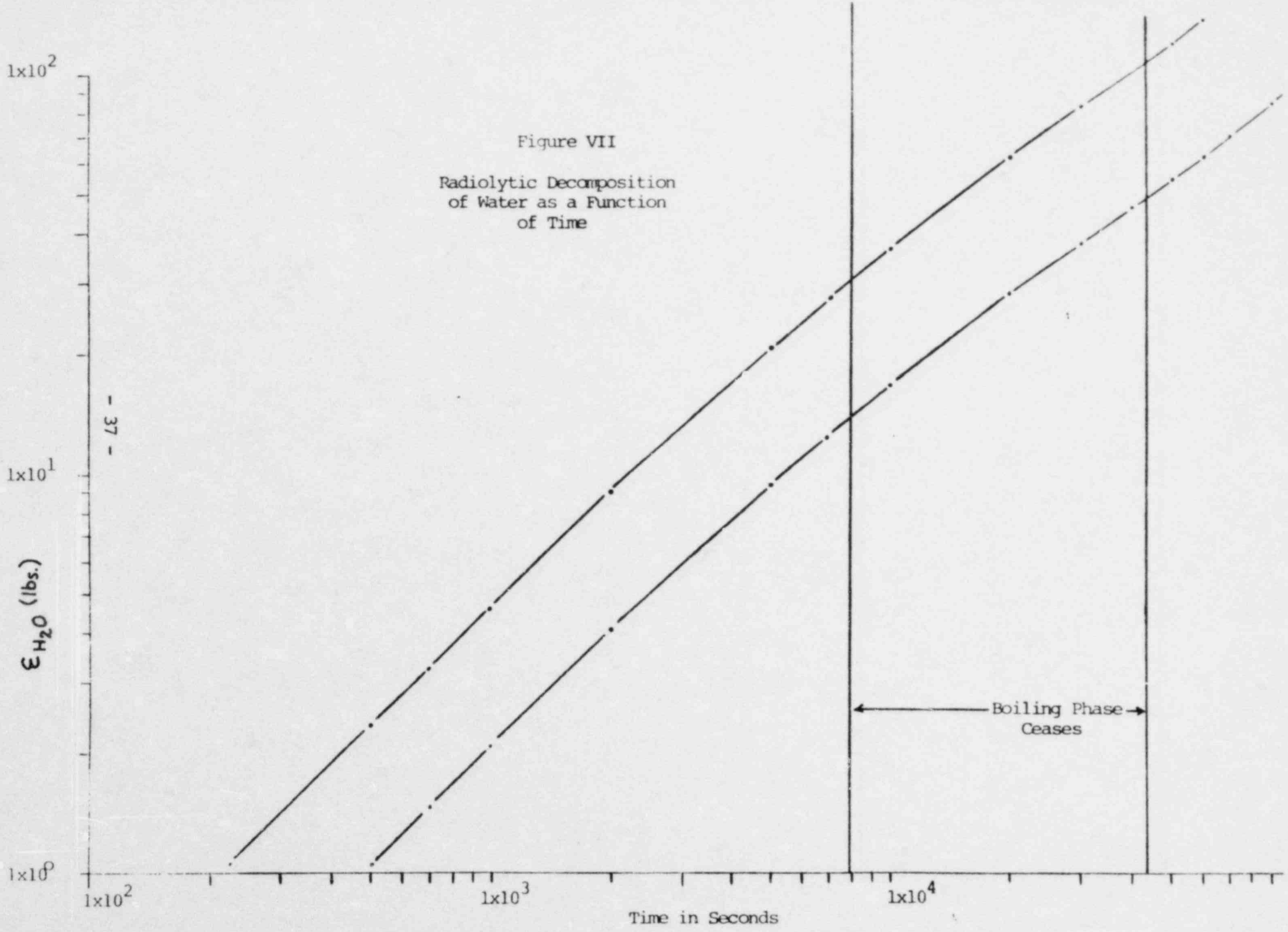


Figure VII

Radiolytic Decomposition of Water as a Function of Time

3.3.2 POST-ACCIDENT GAS CONCENTRATIONS AFTER THE BOILING PHASE

As a result of the postulated metal-water reaction and subsequent radiolytic decomposition of coolant water during the boiling phase, additional hydrogen and oxygen were produced. These additional moles of gas enter the containment atmosphere and a portion will have become dissolved into the torus water (which is subsequently being reinjected into the core via action of the Low Pressure E.C.C.S. Systems). In order to assess post-boiling flammability, and the long-term effects of subcooled radiolysis and recombination, it is necessary to develop an accurate understanding of the gas concentrations both within the torus water and in the containment atmosphere.

Based on information derived in Sections 2.2 and 2.3, it is known that the following initial conditions existed.

Gas Species	Moles of Gas in Containment Atmosphere	Moles of Gas in Torus Inventory*	Net Moles of Gas	Molar Concentration in Torus Inventory
H_2	2.7085×10^{2}	1.936×10^{0}	2.72786×10^{2}	7.433×10^{-7}
O_2	1.0834×10^{4}	1.103×10^{2}	1.09443×10^{4}	4.233×10^{-5}
N_2	2.59745×10^{5}	1.35×10^{3}	2.61095×10^{5}	5.183×10^{-4}

---

*Based on Henry's Law Solubility Limits

The number of moles of H_2 gas generated as a result of the metal-water reaction was shown to be expressed as:

$$\Delta n_{H_2} = 2\, f_{Zr-H_2O}\, n_{Zr} \tag{3.15}$$

The number of moles of H_2 and O_2 generated by boiling phase radiolysis were respectively defined as:

$$\Delta n_{H_2}' = \varepsilon_{H_2O}\, X_{H_2} \qquad X_{H_2} = \frac{25.178 \text{ moles}}{\text{lb. } H_2O} \tag{3.16a}$$

$$\Delta n_{O_2}' = \varepsilon_{H_2O}\, X_{O_2} \qquad X_{O_2} = \frac{12.589 \text{ moles}}{\text{lb. } H_2O} \tag{3.16b}$$

As a result of the analyses and sensitivity studies carried out in Section 3.3.1, it was determined that the upper and lower bounds on ε_{H_2O} were respectively 110 lbs. and 14.0 lbs. H_2O decomposed. This imples that the range in the number of moles of H_2 and O_2 added are between the following values.

Gas Species	Minimum ε_{H_2O} Δn (moles)	Maximum ε_{H_2O} Δn (moles)
H_2	3.5249×10^2	2.7696×10^3
O_2	1.7625×10^2	1.3848×10^3

From a worst case point of view, it may be assumed that all gases generated do not become initially dissolved in the torus water. The ranges of containment gas concentrations will then lie between limit lines defined parametrically for different f_{Zr-H_2O} values as follows:

Upper Limit:

$$[H_2]_c \ (f_{Zr-H_2O}) = \frac{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr} + \text{Max. } \varepsilon_{H_2O}\, X_{H_2}}{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr} + \text{Max. } \varepsilon_{H_2O}\, (X_{H_2} + X_{O_2}) + n_{O_2} + n_{N_2} + n_x} \tag{3.17a}$$

$$[O_2]_c \ (f_{Zr-H_2O}) = \frac{n_{O_2} + \text{Max. } \varepsilon_{H_2O}\, X_{O_2}}{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr} + \text{Max. } \varepsilon_{H_2O}\, (X_{H_2} + X_{O_2}) + n_{O_2} + n_{N_2} + n_x} \tag{3.17b}$$

Lower Limit

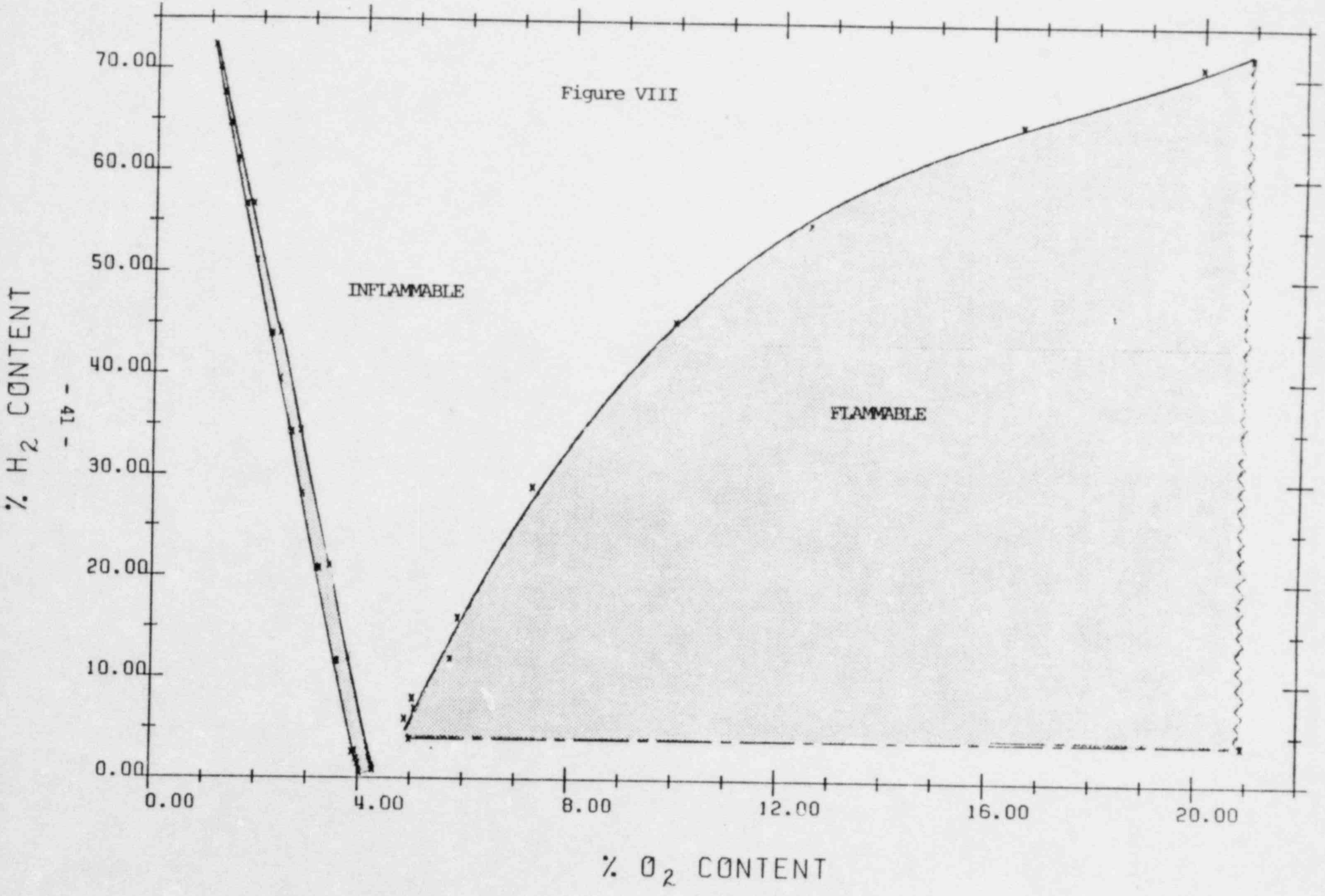
$$[H_2]_c \ (f_{Zr-H_2O}) = \frac{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr} + \text{Min. } \varepsilon_{H_2O}\, X_{H_2}}{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr} + \text{Min. } \varepsilon_{H_2O}\, (X_{H_2} + X_{O_2}) + n_{O_2} + n_{N_2} + n_x} \tag{3.18a}$$

$$[O_2]_c \ (f_{Zr-H_2O}) = \frac{n_{O_2} + \text{Min. } \varepsilon_{H_2O}\, X_{O_2}}{n_{H_2} + 2f_{Zr-H_2O}\, n_{Zr} + \text{Min. } \varepsilon_{H_2O}\, (X_{H_2} + X_{O_2}) + n_{O_2} + n_{N_2} + n_x} \tag{3.18b}$$

A short computer program was written to evaluate these limit lines. A program listing and sample outputs are discussed in Appendix F of Volume II. The results for these calculation are shown in Figure VIII. As can be seen, the region of possible gas concentrations is both sharply defined and sufficiently away from the limits of flammability to alleviate concerns over a short-term H_2 burn.

As a more realistic case, it may be assumed that some portion of the additional generated gases (H_2 and O_2) are distributed

Figure VIII



RANGE OF POSSIBLE POST BOILING PHASE GAS CONCENTRATIONS according to a molar gas/liquid partition coefficient. In this case, the partition coefficient of gas "X" denoted as γ_x would be defined as follows:

$$\gamma_x = \frac{\text{number of moles X in containment gas volume}}{\text{number of moles X dissolved in containment liquid}} \tag{3.19}$$

The number of moles of X in the containment gas volume denoted $(n_x)g$ may be expressed as:

$$(n_x)\ g = \frac{p_x\ V_{cont}}{RT} \tag{3.20}$$

The number of moles of X dissolved in containment liquids may be calculated based on solubility data contained in Volume III. Defining the solubility in 10^{-3} gr/liter H_2O as S_x and m_x as the molecular weight, then:

$$(n_x)_{liq} = [X]V_{liq} = \frac{S_x\ p_x}{m_x}\ V_{liq} \tag{3.21}$$

The partition coefficient may then be defined as:

$$\gamma_x = \frac{m_x}{S_x RT}\ \left(\frac{V_{cont}}{V_{liq}}\right) \tag{3.22}$$

Use of this partition coefficient allows simplified calculations of containment gas concentrations in the following manner:

$$n_x = (n_x)_{liq} + (n_x)g \qquad (3.23)$$

where:

$$(n_x)_{liq} = \frac{1}{\gamma_x + 1} n_x \qquad (3.24a)$$

$$(n_x)_g = \frac{\gamma x}{\gamma_x + 1} n_x \qquad (3.24a)$$

Making use of these definitions, upper and lower limits of H_2 and O_2 following the cessation of core boiling may be defined in the following manner:

Upper Limit:

$$[H_2]_c =$$

$$= \frac{\left(\frac{\gamma_{H_2}}{\gamma_{H_2}+1}\right)[n_{H_2} + 2f_{Zr-H_2O} n_{Zr} + \mathrm{Max}\, \varepsilon_{H_2O} X_{H_2}]}{\left(\frac{\gamma_{H_2}}{\gamma_{H_2}+1}\right)[n_{H_2} + 2f_{Zr-H_2O} n_{Zr} + \mathrm{Max}\, \varepsilon_{H_2O} X_{H_2}] + \left(\frac{\gamma_{O_2}}{\gamma_{O_2}+1}\right)[n_{O_2} + \mathrm{Max}\, \varepsilon_{H_2O} X_{O_2}] + \left(\frac{\gamma_{N_2}}{\gamma_{N_2}+1}\right) n}$$

(3.25a)

$$[O_2]_c =$$

$$= \frac{\left(\frac{\gamma_{O_2}}{\gamma_{O_2}+1}\right)[n_{O_2} + \mathrm{Max}\, \varepsilon_{H_2O} X_{O_2}]}{\left(\frac{\gamma_{H_2}}{\gamma_{H_2}+1}\right)[n_{H_2} + 2f_{Zr-H_2O} n_{Zr} + \mathrm{Max}\, \varepsilon_{H_2O} X_{H_2}] + \left(\frac{\gamma_{O_2}}{\gamma_{O_2}+1}\right)[n_{O_2} + \mathrm{Max}\, \varepsilon_{H_2O} X_{O_2}] + \left(\frac{\gamma_{N_2}}{\gamma_{N_2}+1}\right) n_{N_2}}$$

(3.25b)

Lower Limit:

(same as Equations 3.25a and b with Min. ε_{H_2O} replacing Max. ε_{H_2O}).

In addition to containment gas concentrations, the concentrations of dissolved gases in the containment liquid (in moles/liter) may also be defined as follows:

Upper Limit:

$$[H_2] = \frac{1}{V_{liq.}} \left(\frac{1}{\gamma_{H_2}+1}\right)[n_{H_2} + 2 f_{Zr-H_2O} n_{Zr} + \text{Max } \varepsilon_{H_2O} X_{H_2}] \quad (3.26a)$$

$$[O_2] = \frac{1}{V_{liq.}} \left(\frac{1}{\gamma_{O_2}+1}\right)[n_{O_2} + \text{Max } \varepsilon_{H_2O} X_{O_2}] \quad (3.26b)$$

Lower Limit:

$$[H_2] = \frac{1}{V_{liq.}} \left(\frac{1}{\gamma_{H_2}+1}\right)[n_{H_2} + 2 f_{Zr-H_2O} n_{Zr} + \text{Min } \varepsilon_{H_2O} X_{H_2}] \quad (3.27a)$$

$$[O_2] = \frac{1}{V_{liq.}} \left(\frac{1}{\gamma_{O_2}+1}\right)[n_{O_2} + \text{Min } \varepsilon_{H_2O} X_{O_2}] \quad (3.27b)$$

A short computer program was written to evaluate the anticipated ranges of dissolved gas concentrations (in moles per liter) that will exist following cessation of boiling. A program listing and sample outputs are discussed in Appendix F of Volume II. The results of these calculations are shown in Figures IX and X for gas/liquid equilibrium at 25°C and 100°C respectively.

Figure X

Equilibrium Post-Boiling Phase Dissolved Gas Concentrations

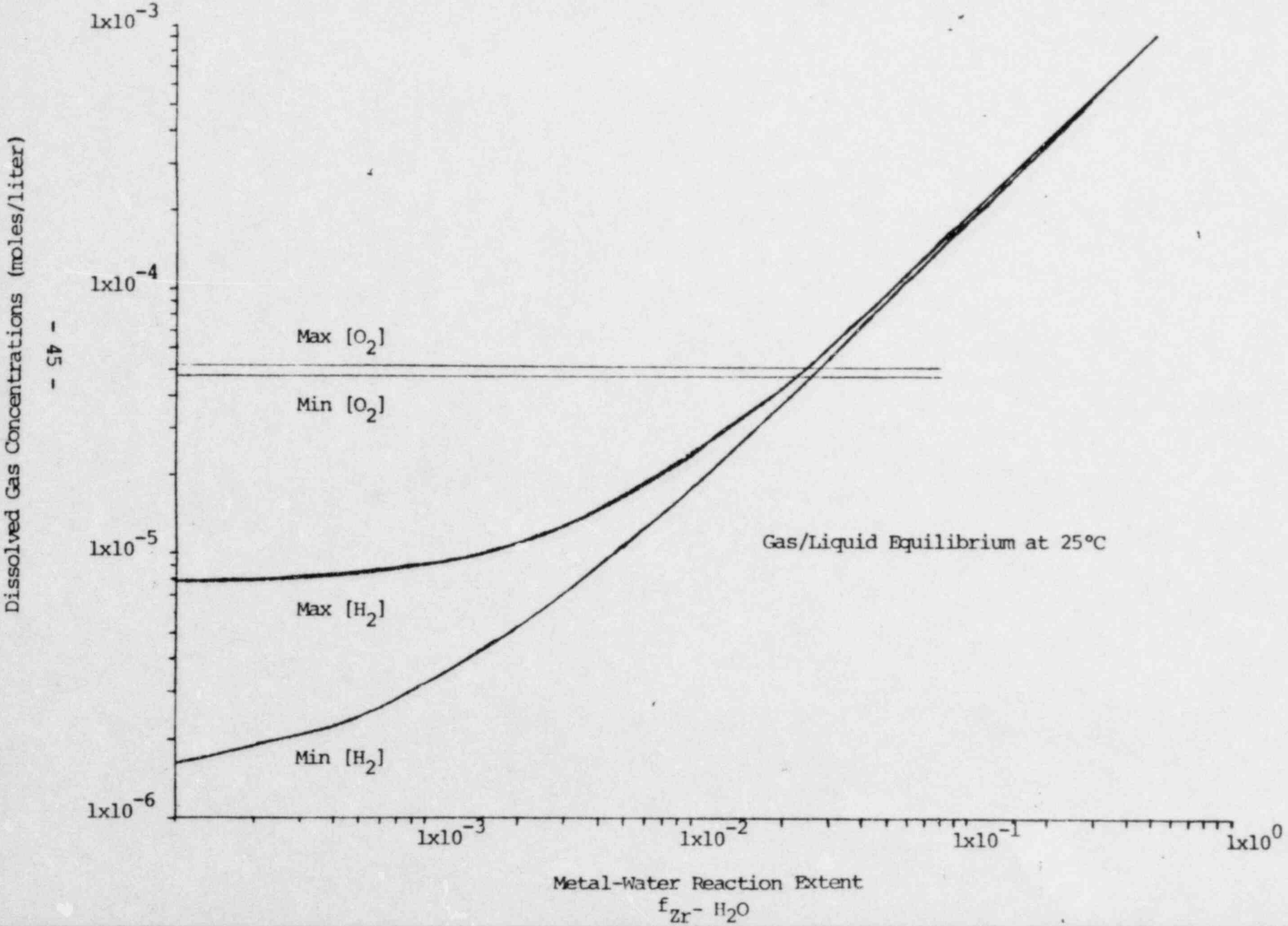
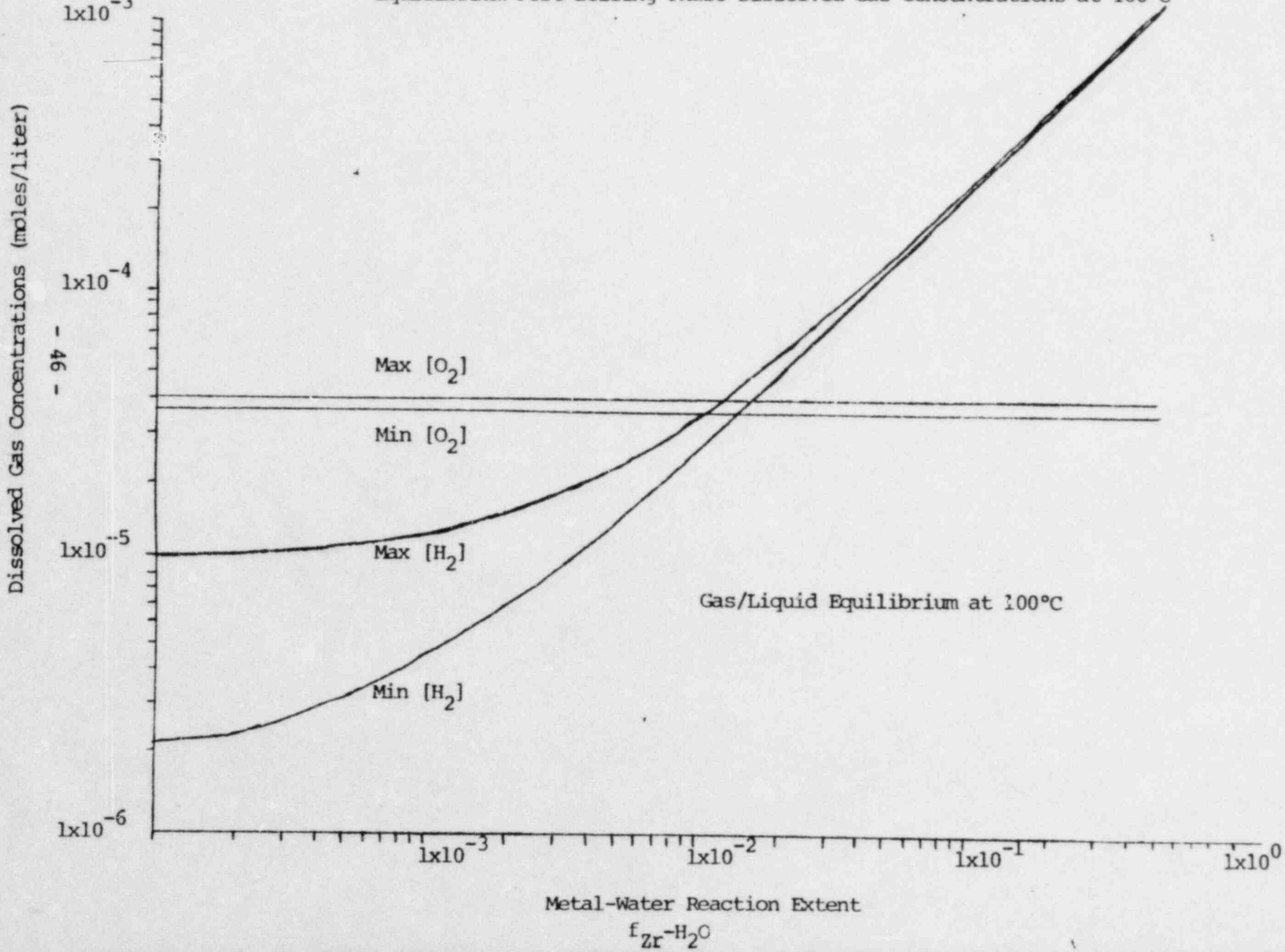


Figure XI

Equilibrium Post-Boiling Phase Dissolved Gas Concentrations at 100°C



CHAPTER 4

DEFINITION OF LONG-TERM HYDROGEN AND OXYGEN SOURCE AND REMOVAL TERMS

4.0 INTRODUCTION

In Chapter 3, the short-term (post-accident boiling phase) hydrogen and oxygen source terms were conservatively defined in terms of the extent of the metal-water reaction and the extent of radiolysis. Based on a conservative analysis of radiolysis during the boiling phase (using methodology similar to that employed in Regulatory Guide 1.7), upper and lower limits on the extent of radiolysis were established based on upper and lower limits of the boiling times determined in Reference 11. Based on Solubility calculations carried out in Section 3.3.2, the existing concentrations (which are parametrically dependent on the extent of metal-water reaction and extent of radiolysis) of H_2 and O_2 at the end of boiling were also determined. These concentrations define the initial conditions for the long-term assessment of radiolysis/recombination effects.

In this chapter, a model is developed for simulation of long-term radiolysis/recombination effects. The use of the computer code FACSIMILE (Flow and Chemical Simulation Code) written and owned by the United Kingdom Atomic Energy Authority is discussed.

4.1 DEVELOPMENT OF A POST-ACCIDENT RADIOLYSIS/RECOMBINATION SYSTEM MODEL

4.1.1 REACTOR SYSTEM CONSIDERATIONS

Dependent on the specific accident scenario involved (e.g., LOCA vs. transient) the post-accident (nonboiling) mode of decay heat removal will involve one of two generic options. Figure XI shows a simplified schematic of the decay heat removal options for a LOCA case. Inventory is maintained via long-term usage of some combination of the low pressure ECC Systems (comprised of 4 Low Pressure Coolant Injection Pumps and 2 Core Spray Pumps). Long-term decay heat removal is accomplished via cooling the injected ECC water in the torus using the Low Pressure Coolant Injection containment spray cooling loops (not shown). The Core Sprays discharge via ring headers at the top of the core, whereas the Low Pressure Coolant Injection trains discharge to the reactor vessel through the recirculation headers. Figure XII shows a simplified schematic of the decay heat removal options for cases where there is an intact reactor coolant system. Inventory can be maintained via cyclic operation of any one of the Low pressure ECC Systems, whereas decay heat removal will be primarily removed via the shutdown cooling systems. (Decay heat removal through the torus represents a secondary albeit more complicated path). In both cases, it is important to recognize that long-term decay heat removal is accomplished via subcooled heat

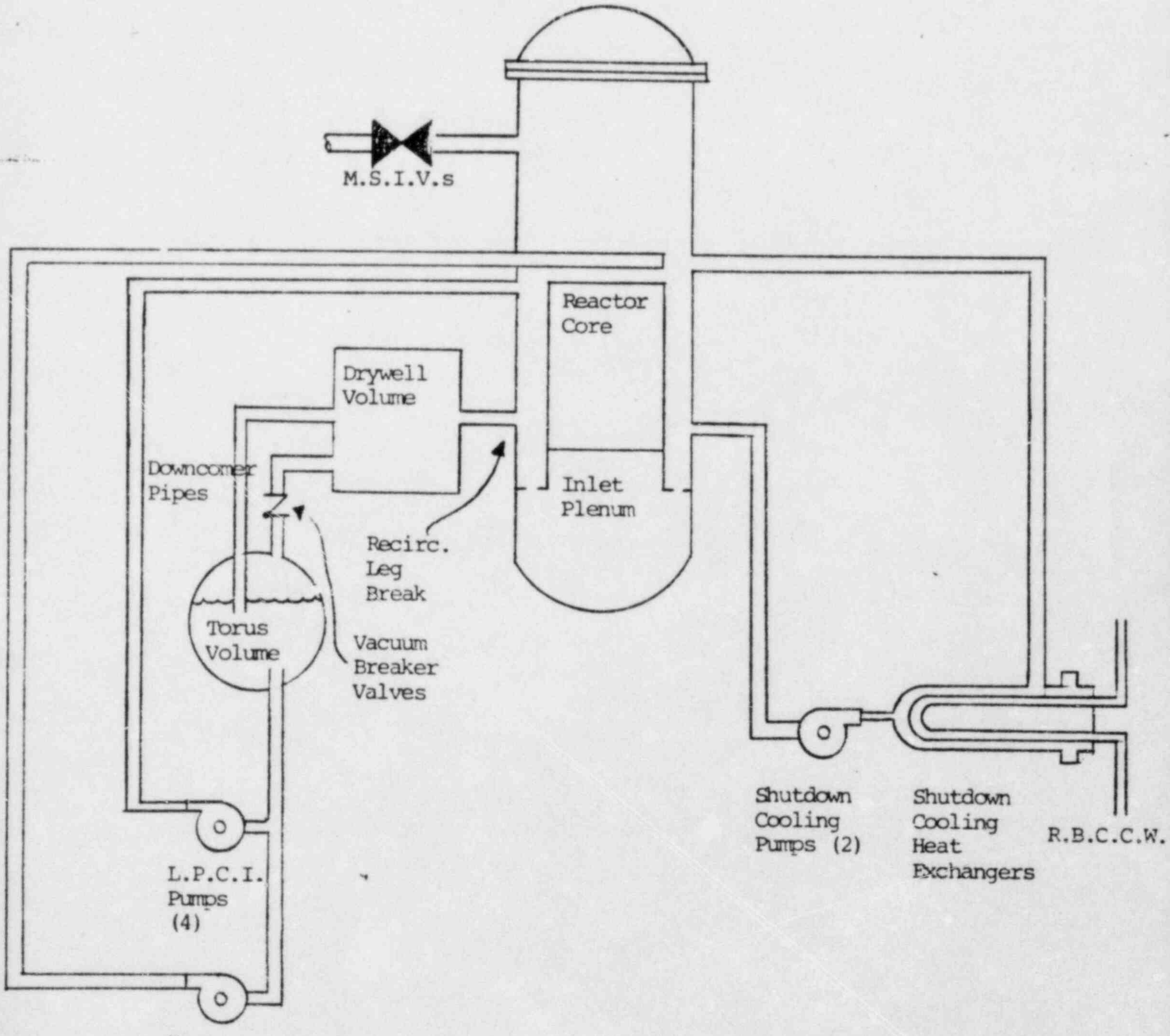


Figure XI

Millstone I Post LOCA Decay Heat Removal Options
-Simplified Schematic-

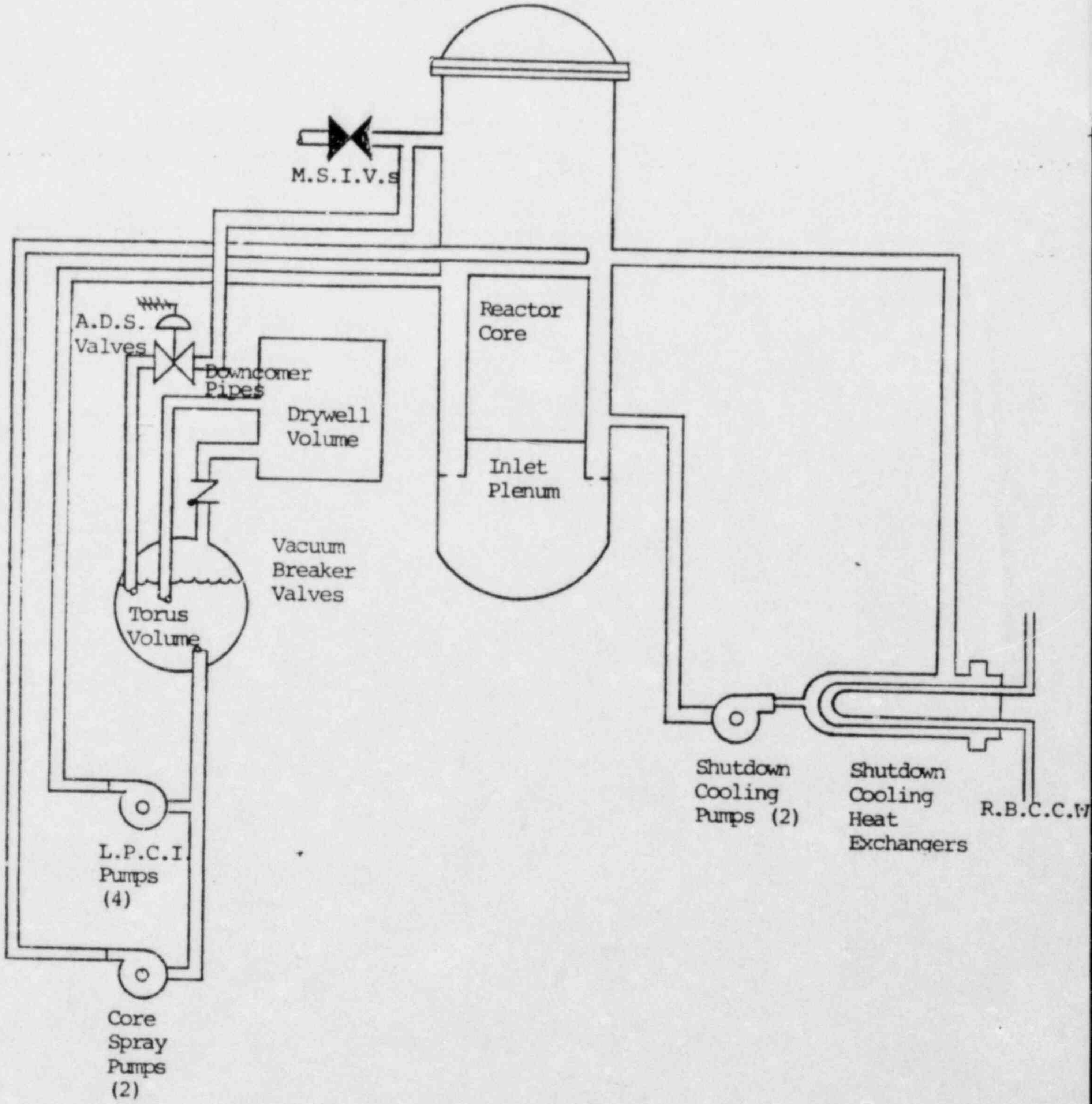


Figure XII

Millstone I Non-LOCA Decay Heat Removal Options
-Simplified Schematic-

transfer processes. Hence, there is no voiding in the core region which could potentially disrupt the chemical recombination effects.

Another significant observation to be drawn from the systems utlizied for long-term decay heat removal is the chemical dilution (or mixing) time constants involved in the injection and bleedoff of coolant from the reactor core. It may be estimated that in the post-accident decay heat removal process a volumetric inventory of 8.0×10^3 to 1.0×10^4 cubic feet of coolant will exist in the core region. The critical time constant for dilution and mixing of the radiolytically induced chemical species in the core volume may be defined as the ratio of the core liquid volume (V_{core}) to the core volumetric flow rate ($\dot{V}_{core}$)

$$T_M = \frac{V_{core}}{\dot{V}_{core}} \qquad (4.1)$$

This time constant may be compared to the time constants for build-up and decay of radiolytically induced species for pure water. Figure XIII shows the build-up of radiolytically induced species, whereas Figure XIV shows the decay (both figures taken from simulations carried out in Reference 15). As shown in these figures only the H_2, O_2, and H_2O_2 species persist for any substantial time period following cessation of radiation (e.g., greater than 1.0 sec.). Hence, water exiting the core (where it has been irradiated) and entering the torus

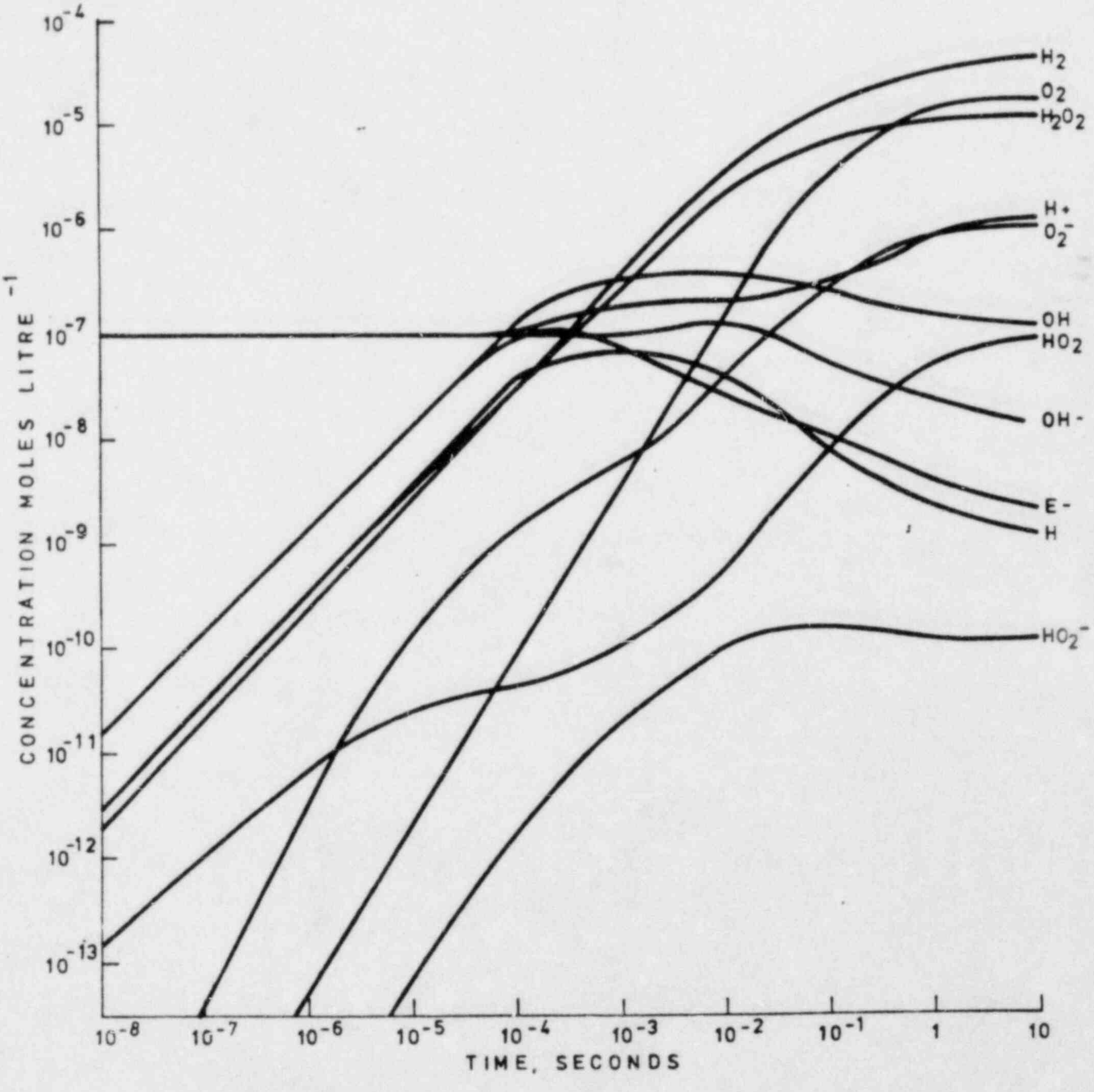


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FIG. XIII βγ RADIOLYSIS (5 WATT GM.$^{-1}$) OF NEUTRAL WATER AT 25°C.

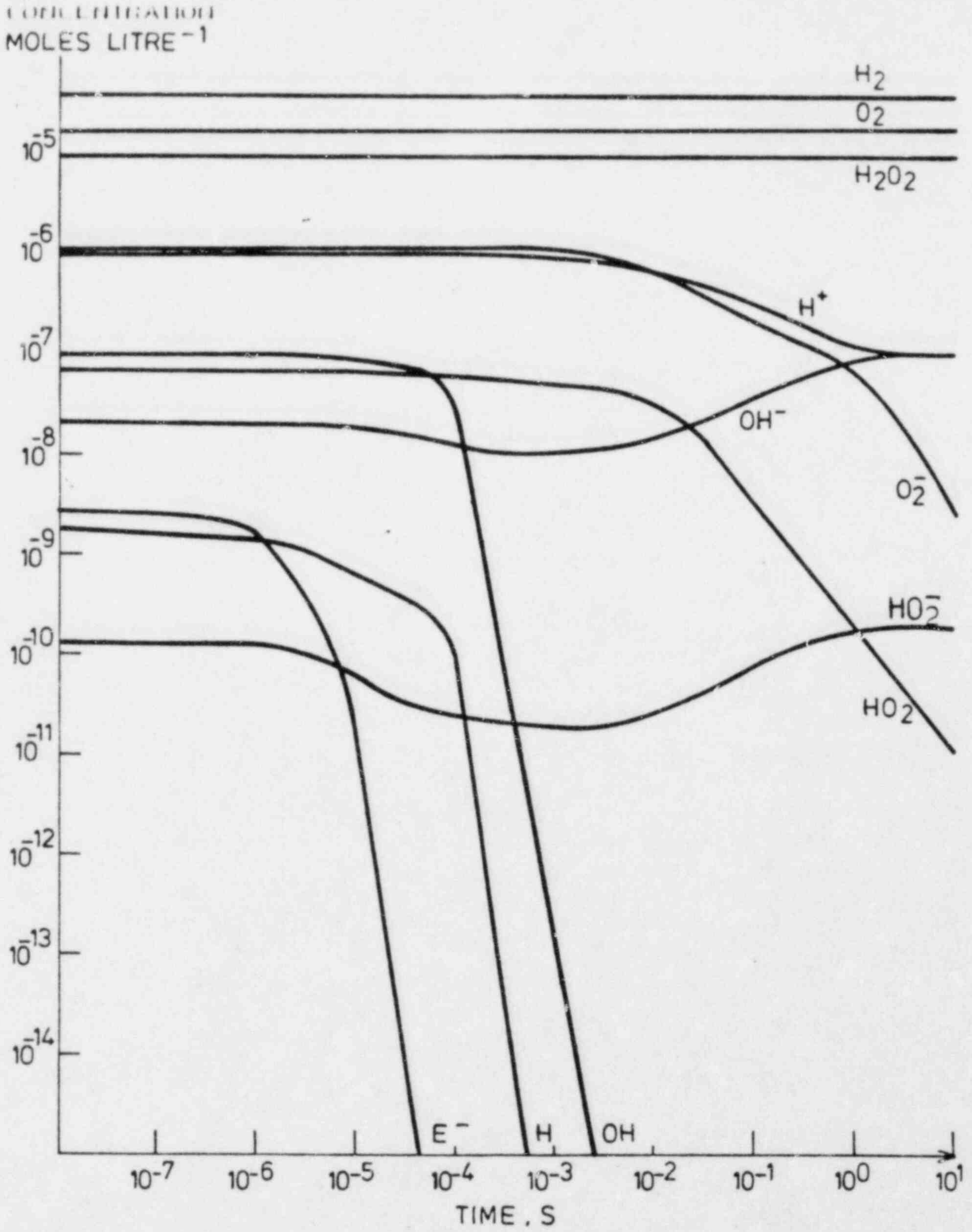

FIG. XIV DECAY OF Bγ RADIOLYSIS PRODUCTS IN PURE WATER AT 25°C.

A.E.R.E. R.8184

region will only contain the species H_2, O_2, and H_2O_2 in any chemically significant quantities. Water entering the core from the torus will similarly only contain the same species. To enter a regime where other radiolytic species would become significant, the volumetric flow rate would have to increase to a level whereby T_M becomes on the order of 1.0 second. Assuming an 8.0×10^3 to 1.0×10^4 cubic foot core inventory this would correspond to flows on the order 8.0×10^3 ft^3/sec. to 1.0×10^4 ft^3/sec. (or 3.59×10^6 gpm to 4.49×10^6 gpm). Clearly, these are orders of magnitude beyond the as-built pumping capablities of the Millstone Unit I decay heat removal systems.

Based on these considerations the noding of the containment model can be accomplished as a three node system with the following features (as summarized in Figure XV).

- Core liquid volume - The initial build-up of radiolytically induced species occurs primarily in this volume. Water containing H_2, O_2, and H_2O_2 concentrations typical of the torus volume are added to this node (proportional to the volumetric flow rate) while water containing H_2, O_2, and H_2O_2 concentrations typical of the radiolytic induced build-up in the core are removed (also at a rate proportional to volumetric flow rate).

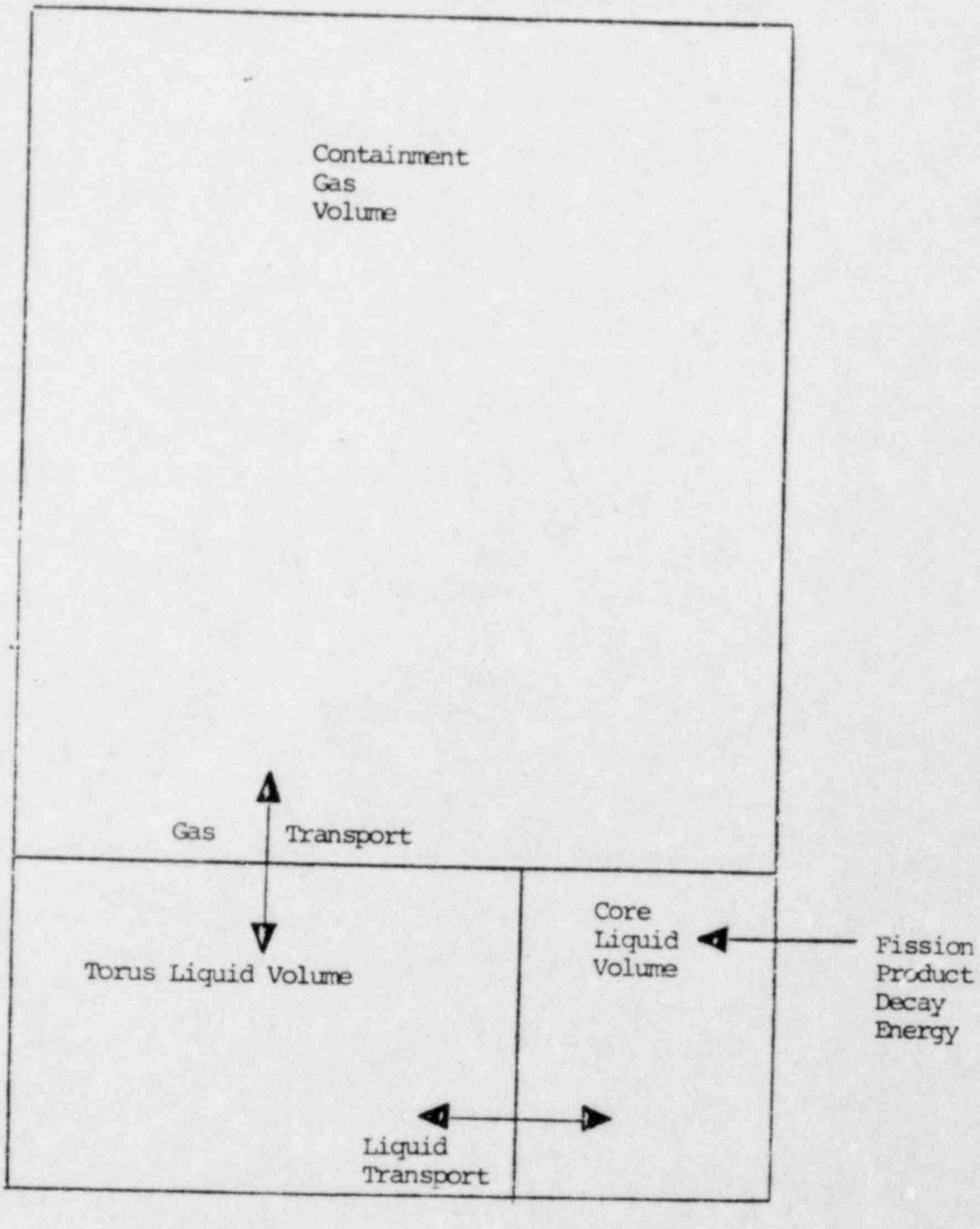

Figure XV

Millstone Unit I Reactor and Containment Noding for Radiolysis/Recombination Simulation

- Torus liquid volume - This volume receives and transfers water from the core liquid volume containing dissolved H_2, O_2, and H_2O_2. H_2 and O_2 transport occurs across the interface of this volume with the containment gas volume. No significant radiolytic induced build-up of species is assumed to occur in this node. Such an assumption is reasonable due to the fact that the dose rate in the core liquid volume is assumed to be many orders of magnitude greater than in the torus region.

- Containment gas volume - This volume receives and transports H_2 and O_2 gas from the torus liquid volume. No leakage of gases is assumed to the Reactor Building due to the fact that this would tend to decrease the potential for flammability.

4.1.2 CHEMICAL KINETICS CONSIDERATIONS

As noted in Section 3.3 the interaction of radiation with water molecules initially results in the prompt generation of a series of free radicals, molecules, and aqueous electrons (e_{aq}, H, H_2, H_2O_2, OH, HO_2) according to initial yields defined in Figure V. The table in Figure XVI summarizes the elementary chemical reactions which occur during the recombination phase based on Reference 15. The specific reactions, rate constants, and activation energies are identical to those defined in References 16, 17, 18, 19 (National Bureau of Standards Data).

In order to formulate a series of homogeneous linear chemical kinetics equations, it must be recognized that the chemical concentration of the various radical and ionic species are affected by the following:

- Introduction of H_2, O_2, and H_2O_2 to the core liquid volume from the torus liquid volume.
- Radiolytic production of various molecular, ionic and radical species based on G value yields.
- Chemical reactions involving the various molecular, ionic and radical species.

FIGURE XVI
RADIOLYTIC DECOMPOSITION AND RECOMBINATION REACTIONS

Chemical Reaction	Rate Constant at 25°C	Activation Energy kcal/mole)
(1) $e_{aq}^- + H_2O \rightarrow H + OH^-$	1.6×10^{1}	3.0
(2) $e_{aq}^- + H^+ \rightarrow H$	2.4×10^{10}	3.0
(3) $e_{aq}^- + OH \rightarrow OH^-$	3.0×10^{10}	3.0
(4) $e_{aq}^- + H_2O_2 \rightarrow OH + OH^-$	1.3×10^{10}	3.0
(5) $H + H \rightarrow H_2$	1.0×10^{10}	3.0
(6) $e_{aq}^- + HO_2 \rightarrow HO_2^-$	2.0×10^{10}	3.0
(7) $e_{aq}^- + O_2 \rightarrow O_2^-$	1.9×10^{10}	3.0
(8) $2e_{aq}^- + \quad \rightarrow 2OH^- + H_2$	5.0×10^{9}	3.0
(9) $2OH \rightarrow H_2O_2$	4.5×10^{9}	3.0
(10) $OH + HO_2 \rightarrow H_2O + O_2$	1.2×10^{10}	3.0
(11) $OH + O_2^- \rightarrow OH^- + O_2$	1.2×10^{10}	3.0
(12) $OH^- + H \rightarrow e_{aq}^- + H_2O$	2.0×10^{7}	3.0
(13) $e_{aq}^- + H + H_2O \rightarrow OH^- + H_2$	4.5×10^{8}	3.0
(14) $e_{aq}^- + HO_2^- + H_2O \rightarrow OH + 2OH^-$	2.0×10^{7}	3.0
(15) $H^+ + OH^- \rightarrow H_2O$	1.4×10^{11}	3.0
(16) $H_2O \rightarrow H^+ + OH^-$	2.6×10^{-5}	3.0
(17) $H + OH \rightarrow H_2O$	2.0×10^{10}	3.0
(18) $OH + H_2 \rightarrow H + H_2O$	4.5×10^{7}	7.0
(19) $OH + H_2O_2 \rightarrow H_2O + HO_2$	4.5×10^{7}	4.5
(20) $H + H_2O_2 \rightarrow OH + H_2O$	9.0×10^{7}	4.5
(21) $H + O_2 \rightarrow HO_2$	1.9×10^{10}	3.0
(22) $HO_2 \rightarrow O_2^- + H^+$	8.0×10^{5}	3.0

Chemical Reaction	Rate Constant at 25°C	Activation Energy kcal/mole)
(23) $O_2^- + H^+ \rightarrow HO_2$	5.0×10^{10}	3.0
(24) $HO_2 + O_2^- \rightarrow O_2 + HO_2^-$	1.5×10^{7}	4.5
(25) $2HO_2 \rightarrow H_2O_2 + O_2$	2.7×10^{6}	4.5
(26) $O_2^- + O_2 \rightarrow H_2O_2 + O_2 + 2OH^-$	less than 10^{2}	4.5
(27) $H + HO_2 \rightarrow H_2O_2$	2.0×10^{10}	3.0
(28) $H + O_2^- \rightarrow HO_2^-$	2.0×10^{10}	3.0
(29) $e_{aq}^- + O_2^- \rightarrow HO_2^- + OH^-$	1.3×10^{10}	4.5
(30) $OH^- + H_2O_2 \rightarrow HO_2^- + H_2O$	1.0×10^{8}	4.5
(31) $HO_2^- + H_2O \rightarrow OH^- + H_2O_2$	1.022×10^{4}	3.0

- Transport of coolant containing H_2O_2, dissolved H_2, and O_2, from the core liquid volume to the torus liquid volume.

- Transport of H_2 and O_2 gas from the containment gas volume to the coolant in the torus liquid volume.

- Removal of dissolved H_2 and O_2 gas from the coolant in the torus liquid volume via transport to the containment gas volume.

The introduction of H_2O_2, H_2, and O_2 into the core liquid volume from the torus liquid volume in governed by the following equations:

$$\frac{d}{dt}[H_2O_2] = [H_2O_2]_T \left(\frac{V_{core}}{\dot{V}_{core}} \right) \qquad (4.2a)$$

$$\frac{d}{dt}[H_2] = [H_2]_T \left(\frac{V_{core}}{\dot{V}_{core}} \right) \qquad (4.2b)$$

$$\frac{d}{dt}[O_2] = [O_2]_T \left(\frac{V_{core}}{\dot{V}_{core}} \right) \qquad (4.2c)$$

-where [X] denotes the molar concentrations in the core liquid volume, $[X]_T$ denotes the molar concentrations in the torus, and $\dot{V}_{core}$ is the volumetric flow rate in liters/sec., and V_{core} is the core liquid volume.

The radiolytic production rate for species "X" may be defined:

$$\frac{d}{dt}[X] = \frac{P_o E_{\beta,\gamma}(t) G_x}{A_o V_{core}} \qquad (4.3)$$

- where:

P_o is the initial core power level (in M_{W_t}).

G_x is the initial yield from radiolysis in molecules per 100eV absorbed dose.

V_{core} is the core region liquid volume, 2.548×10^5 liters is assumed.

$E_{\beta,\gamma}(t)$ is the β, γ energy decay curve previously defined in Equation 3.13 in Chapter 3.

$$E_{\beta,\gamma}(t) = f_{\beta,\gamma} K_o \sum_i k_i e^{-\lambda_i t} \qquad (4.3)$$

A_o is Avogadro's number 6.023×10^{23} per mole.

The effects of gas transport to and from the torus liquid volume from the containment gas volume may be modelled by noting the following rate law:

$$\frac{d}{dt}[X]_T = \frac{1}{V_{torus}} \frac{dn_x}{dt} = \text{Rate (to liquid)} - \text{Rate (from liquid)} \tag{4.5}$$

The Rate of Transport to liquid in the torus (in Equation 4.5) may be determined by noting that the rate of transport varies with the partial pressure of gas within the containment volume.

$$\frac{1}{V_{torus}} \frac{dn_x}{dt} = \frac{1}{RT} \frac{dp_x}{dt} \left(\frac{V_{cont}}{V_{torus}} \right) \tag{4.6}$$

The rate at which the gas partial pressure in the containment gas volume can change is proportional to the product of the rate constant $k_T(X)$ and p_x, hence:

$$\frac{1}{V_{torus}} \frac{dn_x}{dt} = \frac{1}{RT} \left(\frac{V_{cont}}{V_{torus}} \right) k_T(X)\, p_x \tag{4.7}$$

The Rate of Removal from liquid (in Equation 4.5) may be determined by noting that the rate of removal varies with the molar chemical concentration in the liquid: $[X]_T$.

$$\frac{1}{V_{torus}} \frac{dn_x}{dt} = k_R(X)\, [X]_T \tag{4.8}$$

Hence, the net equation defining $[X]_T$ independent of other source and sink effects would be as follows:

$$\frac{d}{dt}[X]_T = \frac{1}{RT} \left(\frac{V_{cont}}{V_{torus}} \right) k_T(X)\, p_x - k_R(X)\, [X]_T \tag{4.9}$$

The equilibrium concentration of X may be defined by noting that when:

$$\frac{d}{dt}[X]_T \equiv 0 \qquad (4.10a)$$

$$[X]_T = \frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)\frac{k_T(X)}{k_R(X)}\,p_X \qquad (4.10b)$$

Specific values of $k_T(X)$ and $k_R(X)$ can be chosen that are analogous to Henry's Law of Solubility (from the solubility data in Volume III).

$$\frac{[X]_T}{p_X} = \frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)\frac{k_T(X)}{k_R(X)} = \frac{S_X}{m_X} \qquad (4.11)$$

Hence, for a given $k_T(X)$:

$$k_R(X) = \frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)\frac{m_X\, k_T(X)}{S_X} \qquad (4.12)$$

- where:

m_X is the atomic (or molecular) weight in grams/mole, S_X is the solubility in 10^{-3} gr/liter H_2O.

The rate of removal of H_2O_2, H_2, and O_2 from the core liquid volume (and transport to the torus liquid volume is governed by the following equations.

$$\frac{d}{dt}[H_2O_2] = -[H_2O_2]\left(\frac{V_{core}}{\dot{V}_{core}}\right) \qquad (4.13a)$$

$$\frac{d}{dt}[H_2] = -[H_2]\left(\frac{V_{core}}{\dot{V}_{core}}\right) \qquad (4.13b)$$

$$\frac{d}{dt}[O_2] = -[O_2]\left(\frac{V_{core}}{\dot{V}_{core}}\right) \qquad (4.13c)$$

The treatment of the effects of chemical reactions assume linearized homogeneous chemical kinetic rate laws (Reference 20).

Taking all of these factors into account, the net behavior of the various species is summarized by the following rate laws:

- Molecular hydrogen, H_2:

$$\frac{d}{dt}[H_2] = \frac{P_0 E_{\beta,\gamma}(t)}{A_0 V_{core}} G_{H_2} + k_5[H]^2 + k_8[e_{aq}^-]^2 + k_{13}[H][e_{aq}^-] - k_{18}[H_2][OH] + ([H_2]_T - [H_2])\frac{V_{core}}{\dot{V}_{core}} \qquad (4.14a)$$

$$\frac{d}{dt}[H_2]_T = ([H_2]-[H_2]_T)\frac{V_{core}}{\dot{V}_{core}} + \frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)(k_T(H_2)\rho_{H_2}) - k_R(H_2)[H_2]_T \qquad (4.14b)$$

- Molecular oxygen, O_2:

$$\frac{d}{dt}[O_2] = k_{10}[OH][HO_2] + k_{11}[OH][O_2^-] + k_{24}[HO_2][O_2^-] + k_{25}[HO_2]^2 + k_{26}[O_2^-]^2 - k_7[e_{aq}^-][O_2] - k_{21}[H][O_2] + ([O_2]_T - [O_2])\frac{V_{core}}{\dot{V}_{core}} \qquad (4.15a)$$

$$\frac{d}{dt}[O_2]_T = ([O_2]-[O_2]_T)\frac{V_{core}}{\dot{V}_{core}} + \frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)k_T(O_2)p_{O_2} - k_R(O_2)[O_2]_T \qquad (4.15b)$$

- Aqueous electron, e_{aq}^-:

$$\frac{d}{dt}[e_{aq}^-] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_{e_{aq}^-} - k_1[e_{aq}^-] - k_2[e_{aq}^-][H^+]$$
$$-k_3[e_{aq}^-][OH] - k_4[e_{aq}^-][H_2O_2] - k_6[e_{aq}^-][HO_2]$$
$$-k_7[e_{aq}^-][O_2] - 2k_8[e_{aq}^-]^2 - k_{13}[e_{aq}^-][H]$$
$$-k_{14}[e_{aq}^-][HO_2^-] - k_{29}[e_{aq}^-][O_2^-] \qquad (4.16)$$

- Atomic hydrogen, H:

$$\frac{d}{dt}[H] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_H + k_1[e_{aq}^-] + k_2[e_{aq}^-][H^+]$$
$$+k_{18}[OH][H_2] - 2k_5[H]^2 - k_{12}[H][OH^-]$$
$$-k_{13}[e_{aq}^-][H] - k_{17}[H][OH] - k_{20}[H][H_2O_2]$$
$$-k_{21}[H][O_2] - k_{27}[H][HO_2] - k_{28}[H][O_2^-] \qquad (4.17)$$

- Hydrogen peroxide, H_2O_2:

$$\frac{d}{dt}[H_2O_2] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_{H_2O_2} + k_9[OH]^2 + k_{26}[O_2^-]^2$$
$$+k_{27}[H][HO_2] + k_{31}[HO_2^-] - k_4[e_{aq}^-][H_2O_2]$$
$$-k_{19}[OH][H_2O_2] - k_{20}[H][H_2O_2] - k_{30}[OH^-][H_2O_2]$$
$$+ ([H_2O_2]_T - [H_2O_2])\frac{V_{core}}{\dot{v}_{core}} \qquad (4.18a)$$

$$\frac{d}{dt}[H_2O_2]_T = ([H_2O_2] - [H_2O_2]_T)\frac{V_{core}}{\dot{v}_{core}} \qquad (4.18b)$$

- Hydroxide radical, OH:

$$\frac{d}{dt}[OH] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_{OH} + k_4[e_{aq}^-][H_2O_2] + k_{14}[e_{aq}^-][HO_2^-]$$
$$+k_{20}[H][H_2O_2] - k_3[e_{aq}^-][OH] - 2k_9[OH]^2$$
$$-k_{10}[OH][HO_2] - k_{11}[OH][O_2^-] - k_{17}[H][OH]$$
$$-k_{18}[OH][H_2] - k_{19}[OH][H_2O_2] \qquad (4.19)$$

- Hydroxide ion, OH^-:

$$\frac{d}{dt}[OH^-] = k_1[e_{aq}^-] + k_3[e_{aq}^-][OH] + k_4[e_{aq}^-][H_2O_2] + k_8[e_{aq}^-]^2 + k_{11}[OH][O_2^-]$$
$$+k_{13}[e_{aq}^-][H] + k_{14}[e_{aq}^-][HO_2^-] + k_{16}[H_2O] + k_{26}[O_2^-]^2$$
$$+k_{29}[e_{aq}^-][O_2^-] + k_{31}[HO_2^-] - k_{12}[OH^-][OH] - k_{15}[H^+][OH^-]$$
$$- k\ [OH^-][H_2O_2]$$

- Perhydroxyl radical, HO_2:

$$\begin{aligned}\frac{d}{dt}[HO_2] = {} & \frac{P_0 E_{\beta,\gamma}(t)}{A_0 V_{core}} G_{HO_2} + k_{19}[OH][H_2O_2] + k_{21}[H][O_2] \\ & + k_{23}[O_2^-][H^+] - k_6[e_{aq}^-][HO_2] - k_{10}[OH][HO_2] \\ & - k_{22}[HO_2] - k_{24}[HO_2][O_2^-] - 2k_{25}[HO_2]^2 \\ & - k_{27}[H][HO_2]\end{aligned} \tag{4.21}$$

- Perhydroxyl ion, HO_2^-:

$$\begin{aligned}\frac{d}{dt}[HO_2^-] = {} & k_6[e_{aq}^-][HO_2] + k_{24}[HO_2][O_2^-] + k_{28}[H][O_2^-] \\ & + k_{29}[e_{aq}^-][O_2^-] + k_{30}[OH^-][H_2O_2] - k_{14}[e_{aq}^-][HO_2^-] \\ & - k_{31}[HO_2^-]\end{aligned} \tag{4.22}$$

- Hydrogen ion, H^+:

$$\begin{aligned}\frac{d}{dt}[H^+] = {} & k_{16}[H_2O] + k_{22}[HO_2] - k_6[e_{aq}^-][H^+] + \frac{P_0 E_{\beta,\gamma}(t)}{A_0 V_{core}} G_{H^+} \\ & - k_{15}[H^+][OH^-] - k_{23}[O_2^-][H^+]\end{aligned} \tag{4.23}$$

- Oxide ion, O_2^-:

$$\begin{aligned}\frac{d}{dt}[O_2^-] = {} & k_7[e_{aq}^-][O_2] + k_{22}[HO_2] - k_{11}[OH][O_2^-] \\ & - k_{23}[O_2^-][H^+] - k_{24}[HO_2][O_2^-] - 2k_{26}[O_2^-]^2 \\ & - k_{28}[H][O_2^-] - k_{29}[e_{aq}^-][O_2^-]\end{aligned} \tag{4.24}$$

4.1.3 CHOICE OF AN APPROPRIATE SIMULATION MODEL

To properly simulate the chemical kinetics, several alternate codes were evaluated. At the time of the TMI-2 accident, Knolls Atomic Power laboratory (K.A.P.L.) utilized Bureau of Naval Reactors simulation codes to analyze whether or not combustible mixtures of H_2 and O_2 could build up (Reference 21). In response to NUSCO inquiries over the availability of the simulation codes used in this report, it was learned that the codes are not in the public domain. The use of alternate codes was then reviewed. The Staff of Argonne National Laboratory (ANL) had also provided independent analysis of the TMI-2 Hydrogen bubble concerns (Reference 22) for the Kemeny Commission (Reference 23). This analysis used a modified version of the WR-20 computer code discussed in References 24 and 25. NUSCO performed a preliminary analysis (Reference 26) using WR-20.

In performing the preliminary analyses (Reference 26), the need to obtain a substantially faster running computer code and ability to treat gas transport to and from the torus liquid was identified. WR-20 (Reference 25) was originally written for evaluation of pulse type radiolysis experiments which last for times on the order of milliseconds. The code is sufficiently accurate for modelling short-term experiments but would present severe limitations for evaluating long-term ($> 10^3$ seconds) radiolysis and recombination. What was desired was a code which could provide an accurate representation of short-term kinetic (such as WR-20) but could also be used for evaluating long-term stability, transport of dissolved gases to and from the core, and the transport of gases to and from the torus from the containment gas space, (such as the classified KAPL Codes). Based on NUSCO's review of the available options, the FACSIMILE Code (References 27, 28, and 29), written and owned by the United Kingdom Atomic Energy Authority (U.K.A.E.A.), was selected. NUSCO subsequently obtained an exclusive use purchase of the FACSIMILE Code in May 1982.

4.2 BASE CASE DEFINITION

In order to understand the separate effects which impact radiolytic decomposition and recombination reactions, it is necessary to first define a BASE CASE which embodies a majority of the phenomenon involved. The question of temperature variations and impurity concentrations can then be treated as perturbations from a well-defined steady state.

For the purposes of this analysis, it is noted that the Millstone Unit I Boiling Water Reactor (B.W.R.) utilizes highly purified water that is continually purified (under normal operation) to remove trace impurities which have an adverse impact on corrosion control and plant personnel radiation exposure. Unlike pressurized water reactors (P.W.R.s) which employ numerous chemical additives (Boric Acid, hydrazine, etc.) boiling water reactors operate with clean, essentially neutral pH water. Additionally, unlike the alkaline containment spray additives used in P.W.R.s, B.W.R.s utilize the torus water which has essentially identical water purity as that used for normal core cooling. In view of this, the analysis BASE CASE is a radiolysis/recombination model assuming pure H_2O with excess dissolved H_2 and O_2 gas reflective of specific f_{Zr-H_2O} and ε_{H_2O} values determined in Section 3.3.2 of Chapter 3. The table in Figure XVII summarizes the key input assumptions utlized in the BASE CASE simulation.

FIGURE XVII

Key Input Assumptions Utilized in Base Case

Parameter	Value	Bases
Water Temp.	25°C	-Minimizes the effect of the dominant recombination reaction: $H_2 + OH \longrightarrow H + (H_2O)$
V_{core}	2.5×10^5 liters	-Smaller liquid inventory yields higher average absorbed dose -Decreases core mixing time constant
V_{cont}	7.223×10^6 liters	-Approximate design value
V_{torus}	2.605×10^6 liters	-Tech. Spec. Value
$\dot{v}_{core}$	10,000 gpm	-Mid range value of possible ECCS injection flows
f_{zr-H_2O}	1%	-Slightly greater value than five times DBA metal-water reaction
ε_{H_2O}	110 lbs.	-Maximum boiling time assumption (e.g., equivalent of 12.0 hrs full core boiling)
$P_{H_2}(0)$	0.0339 atmos.	-Corresponds to previously noted f_{zr-H_2O}, ε_{H_2O} values for T = 25°C
$P_{O_2}(0)$	0.041 atmos.	-Corresponds to previously noted f_{zr-H_2O}, ε_{H_2O} values for T = 25°C
$[H_2](0)$	2.63×10^{-2} moles/liter	-Corresponds to previously noted f_{zr-H_2O}, ε_{H_2O} values for T = 25°C
$[O^2](0)$	$5\text{-}15 \times 10^{-5}$ moles/liter	-Corresponds to previously noted f_{zr-H_2O}, ε_{H_2O} values for T = 25°C
$k_T(O_2)$	1.0	-Pure assumption *
$k_T(H_2)$	4.0	-Based on: $\frac{\text{Rate of } H_2 \text{ Diffusion in Gas}}{\text{Rate of } O_2 \text{ Diffusion in Gas}} = \sqrt{\frac{m_{O_2}}{m_{H_2}}}$
$k_R(O_2)$	$\frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)\frac{m_{O_2}k_T(O_2)}{S_{O_2}}$	-Based on Equation 4.12 to assure equilibrium equivalent to Henry's Law Gas Solubility
$k_R(H_2)$	$\frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)\frac{m_{H_2}k_T(H_2)}{S_{H_2}}$	-Based on Equation 4.12 to assure equilibrium equivalent to Henry's Law GAs Solubility

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*Review comments from Dr. K. Schmidt (ANL) indicate this value is $\sim 10^2$ hence the assumed value is quite conservative

Figure XVIII shows the results of the long-term containment gas partial pressure calculations. As is noted in this figure, there is a net continuous recombination of H_2 and O_2 gases initially generated as a result of the metal-water reaction and boiling phase radiolysis. Figure XIX shows the time dependent concentrations of radiolytically induced molecular, ionic, and radical species within the core liquid region. Previous analyses of post-accident hydrogen and oxygen recombination (Reference 22) have shown that the net rate of recombination is sensitive to the rate of gas transport from the gas region to the liquid region. In general, however, the specific values of these constants are unknown. Because of this sensitivity calculations were carried out over a wide range of possible $k_T(H_2)$, $k_T(O_2)$ values. The results of these sensitivity calculations are shown in Appendix G of Volume II. In general these sensitivity calculations show that larger values of $k_T(H_2)$ and $k_T(O_2)$ will increase the rate of recombination but will have no impact on the long-term equilibrium values of P_{H_2} and P_{O_2}.

4.2.1 Evaluation of Sensitivity to Core Flow Rate

Experiments conducted by Zittel (Reference 12) at Oak Ridge National Laboratory (O.R.N.L) indicated a slight sensitivity to the core volumetric flow rate. The chemical kinetics equations all show a linear dependence on core flow rate in the rate at which the torus liquid volume equilibriates with the core liquid volume. Equilibrium between the torus and core volumes essentially defines the equilibrium values (e.g.: $[H_2] = [H_2]_T$).

Figure XVIII

BASE CASE Containment Gas Partial Pressures vs. Time (at 25°C)

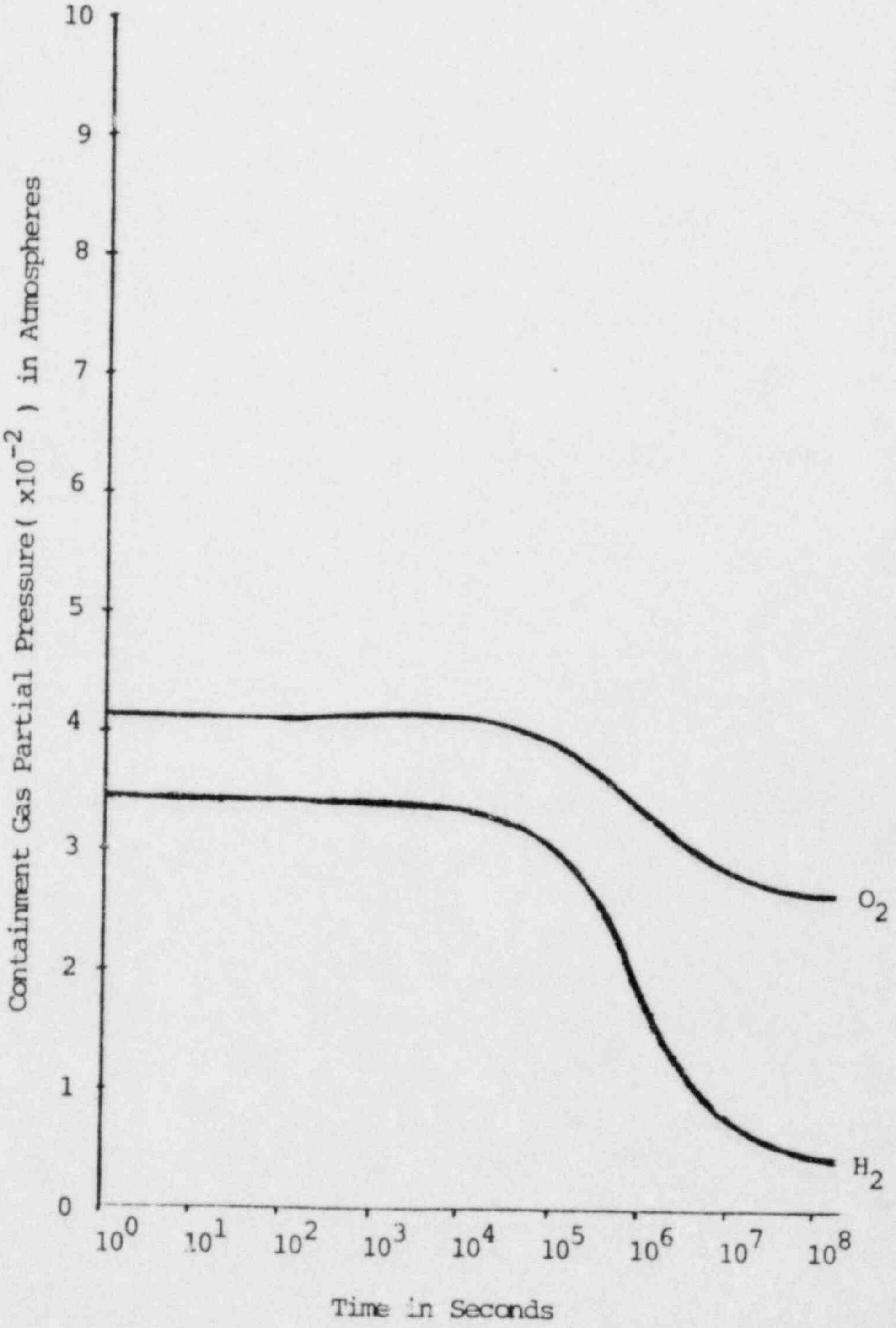
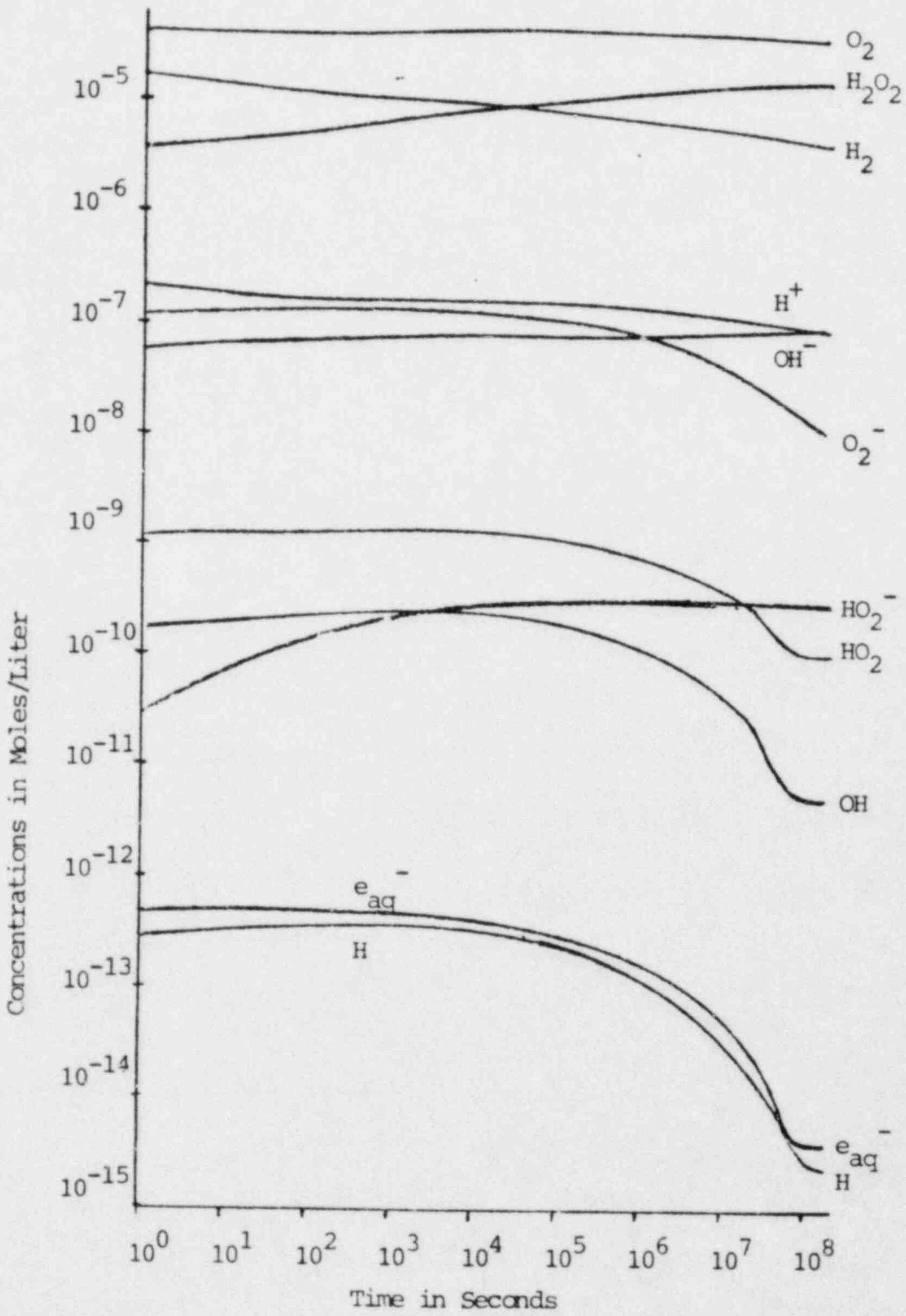


Figure XIX

BASE CASE Time Dependent Concentrations of Radiolytically Induced Species (at 25°C)



To evaluate the dynamic sensitivity to the core volumetric flow rates a series of simulation runs were carried out in which $\dot{V}_{core}$ was varied upwards and downwards by a factor of 10. The results of these calculations are shown in Figure XX. (Computer runs are documented in Appendix H of Volume II). As shown in this figure, increasing the core volumetric flow rate speeds up the rate of recombination, whereas the equilibrium values of $[H_2]$ and $[O_2]$ are unaffected.

4.2.2 Evaluation of Sensitivity to Extent of Zr-H_2O Reaction

Clearly a major factor promoting the net continuous recombination of the H_2 with O_2 in the containment is the excess H_2 present as a result of the assumed Zr-H_2O reaction. The BASE CASE initial conditions for P_{O_2} and P_{H_2} were chosen to simulate slightly more than the five times DBA f_{Zr-H_2O} value. In order to assure the widest possible range of "safe" post-accident conditions within the containment it is necessary to examine the sensitivity of the BASE CASE results to the chosen value of the extent of the Zr-H_2O reaction: f_{Zr-H_2O}.

The minimal possible initial H_2 overpressure would be for the case where: $f_{Zr-H_2O} = 0.0$. In this case the only significant source of H_2 is from boiling phase radiolysis. Figure XXI shows the results of the containment gas partial pressure analysis for $f_{Zr-H_2O} = 0.0$. As noted in this figure there is

Figure XX

BASE CASE SENSITIVITY TO CORE VOLUMETRIC FLOW RATE

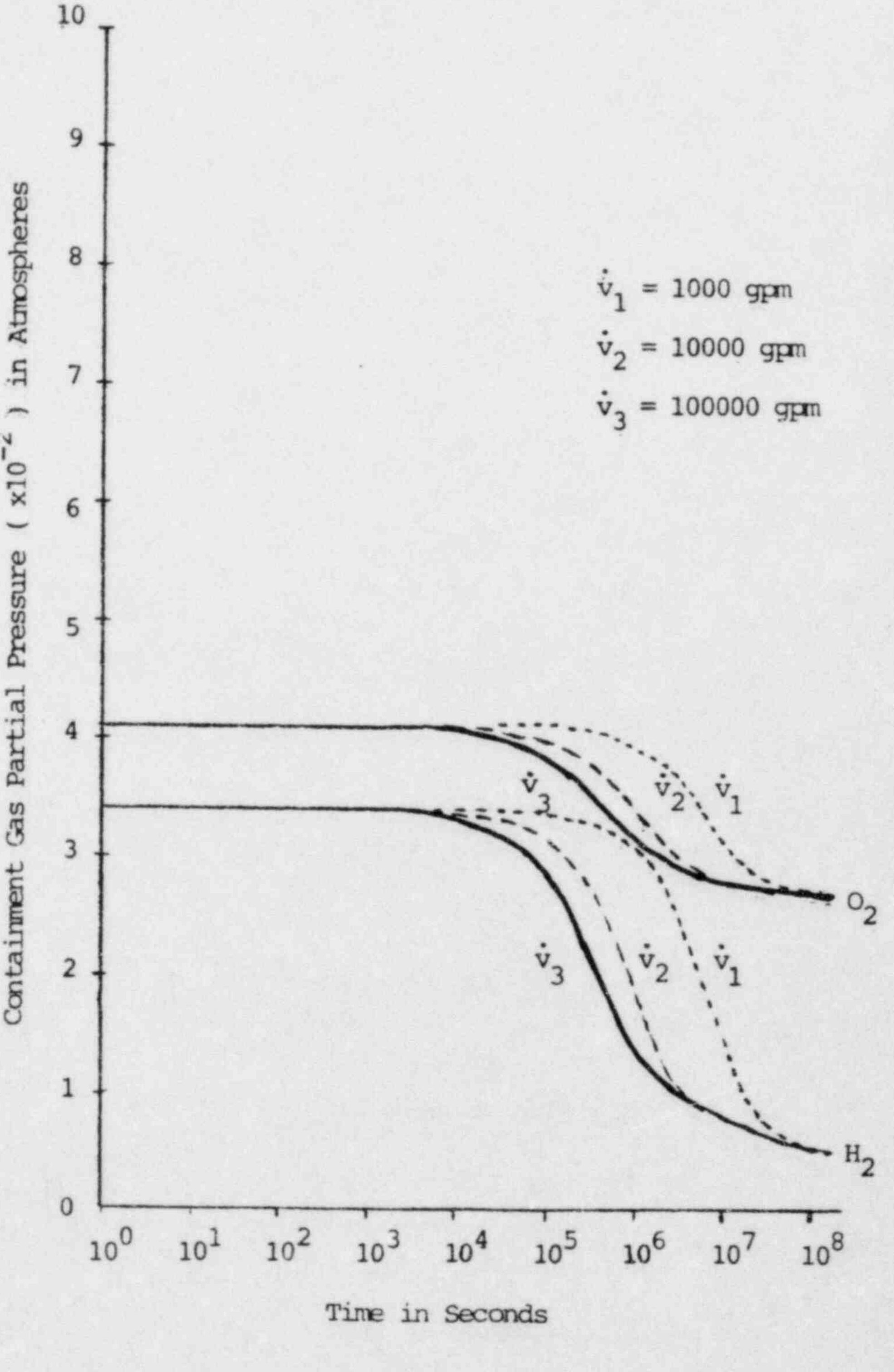
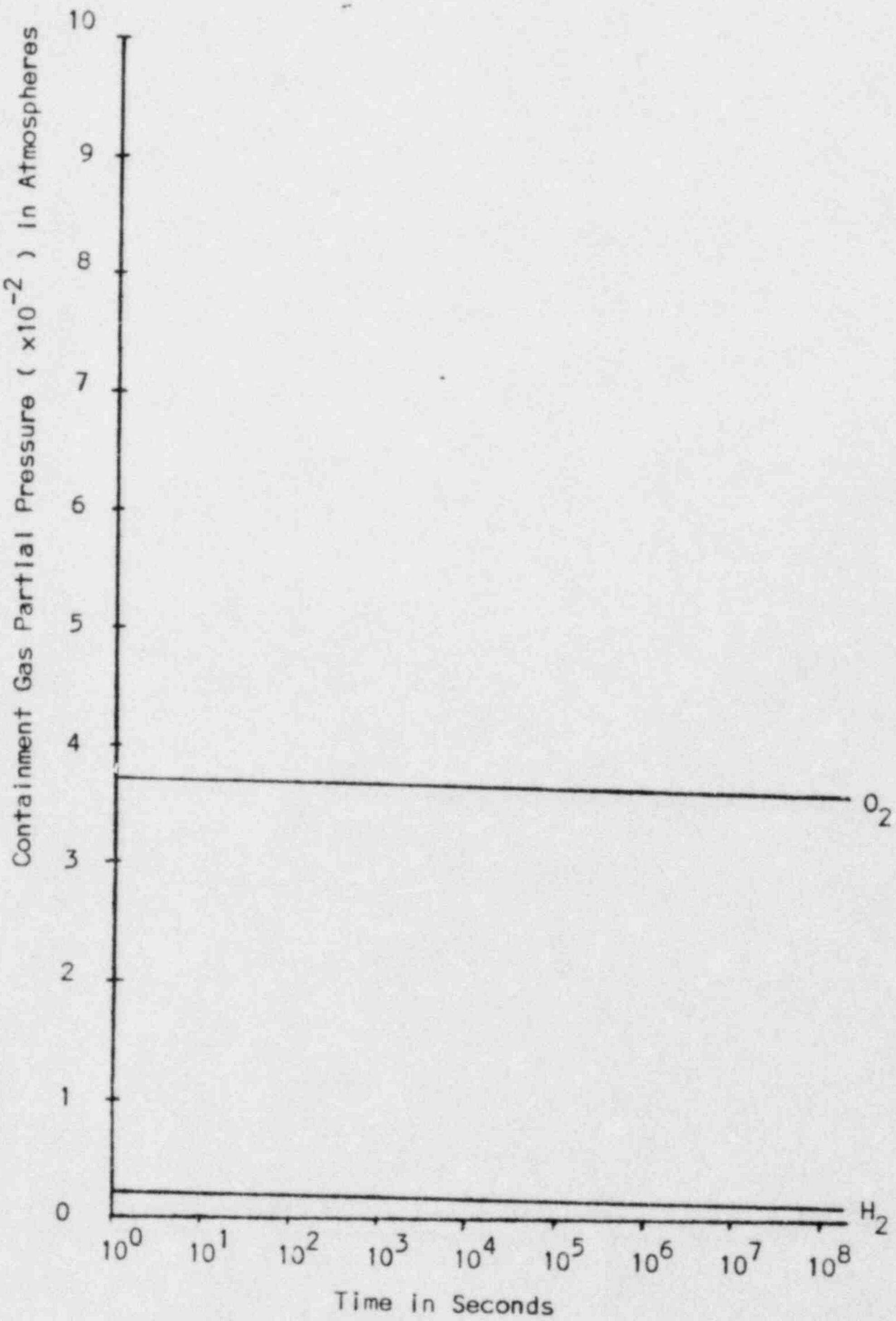


Figure XXI

BASE CASE Sensitivity to Extent of Zr-H_2O Reaction



only a slight decrease in P_{H_2} and P_{O_2} as long-term equilibrium values are attained.

An additional case of interest is the limiting Millstone Unit I f_{Zr-H_2O} value determined in Section 3.2 (e.g.: $f_{zr-H_2O} = 0.00612$). The results of this simulation are essentially identical to the $f_{Zr-H_2O} = 0$ case. (The FACSIMILE Simulations for these cases are documented in Appendix I of Volume II.)

4.2.3 EVALUATION OF TEMPERATURE SENSITIVITY

Temperature effects equilibrium levels of dissolved H_2 and O_2 in two ways:

- gas solubility is temperature dependent, hence $k_T(X)$ and $k_R(X)$ will vary as a function of the water temperature

- the rates of chemical reactions occurring during the recombination phase are temperature dependent (increasing temperature increases the chemical reaction rates)

The variation in gas solubility is treated in this analysis by adjusting the solubility using the data found in Volume III.

Adjustment of the chemical reaction rates for different water temperatures may be accomplished via Arrhenius' Law which states that the rate of a chemical reaction (or: $k_i(T)$) varies with temperature as follows:

$$k_i(T) = A_i e^{-E_i/RT} \tag{4.25}$$

where: A_i is a proportionality constant

E_i is the activation energy in cal./mole

R is the Gas Law constant,

$$R = .08205 \; \frac{\text{liter} \cdot \text{atmospheres}}{\text{mole} \cdot {}^\circ\text{K}}$$

T is the absolute temperature in °K.

All of the basic chemical reactions shown previously in Figure XI have rate constants experimentally measured at 25°C (298.15°K or 77°F). These constants may be extrapolated to higher temperature values by noting the ratio of rate constants for two different temperatures is:

$$\frac{k_i(T)}{k_i(T_o)} = \frac{A_i e^{-E_i/RT}}{A_i e^{-E_i/RT}}$$

$$= e^{-E_i/R \, (\frac{1}{T} - \frac{1}{T_o})} \tag{4.26}$$

Hence:

$$k_i(T) = k_i(T_o)e^{-E_i/R\left(\frac{1}{T} - \frac{1}{T_o}\right)} \qquad (4.27)$$

To extrapolate the rate constants for water temperatures of 25°C, 50°C, 75°C, 100°C (respectively: 298.15°K, 323.15°K, 348.15°K, and 373.15°K) a short computer program was written. This program and the results are shown in Appendix J of Volume II. Using these temperature dependent values the BASE CASE was re-evaluated. Figures XXII and XXIII show the results of these comparisons. (FACSIMILE simulations are also documented in Appendix J of Volume II).

4.3 EFFECTS OF FISSION PRODUCT AND CHEMICAL IMPURITIES

Section 4.2 evaluated a BASE CASE which assumed essentially pure (neutral pH) water with excess dissolved H_2 and O_2. Numerous researchers in the past have noted the potential impacts of impurities on the recombination rate. The potential mechanism by which impurities can alter the recombination rate is by removal of H and OH radicals which are necessary to recombine the H_2 and O_2, via oxidation and reduction reactions. This potential exists because of the fact OH is a strong oxidizing agent, whereas H is a strong reducing agent. Denoting a typical halide impurity as: M^-, the effects of this impurity in the water can be summarized via the following half-cell reactions.

Figure XXII

Containment Gas Partial Pressures vs. Time (at 100°C)

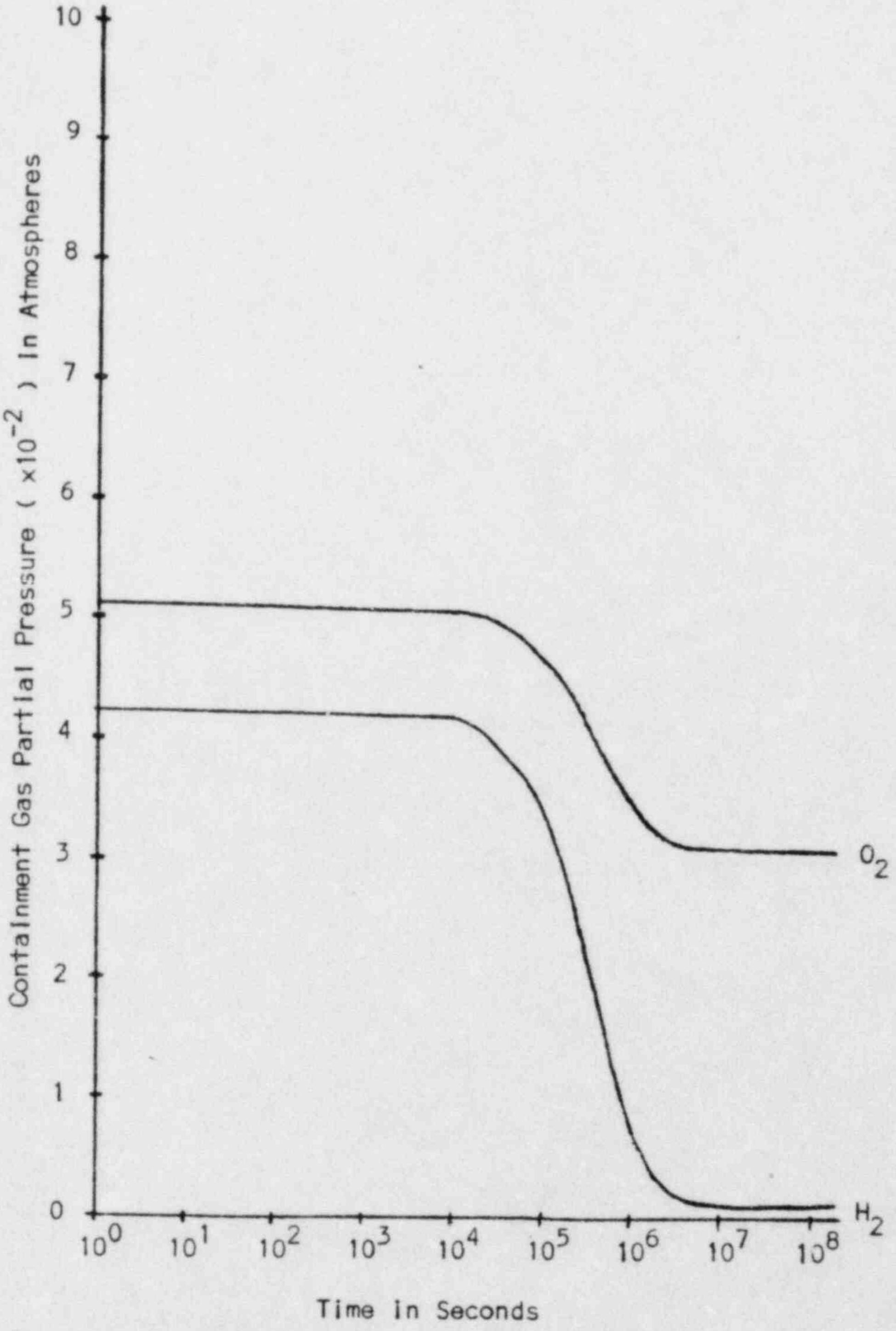
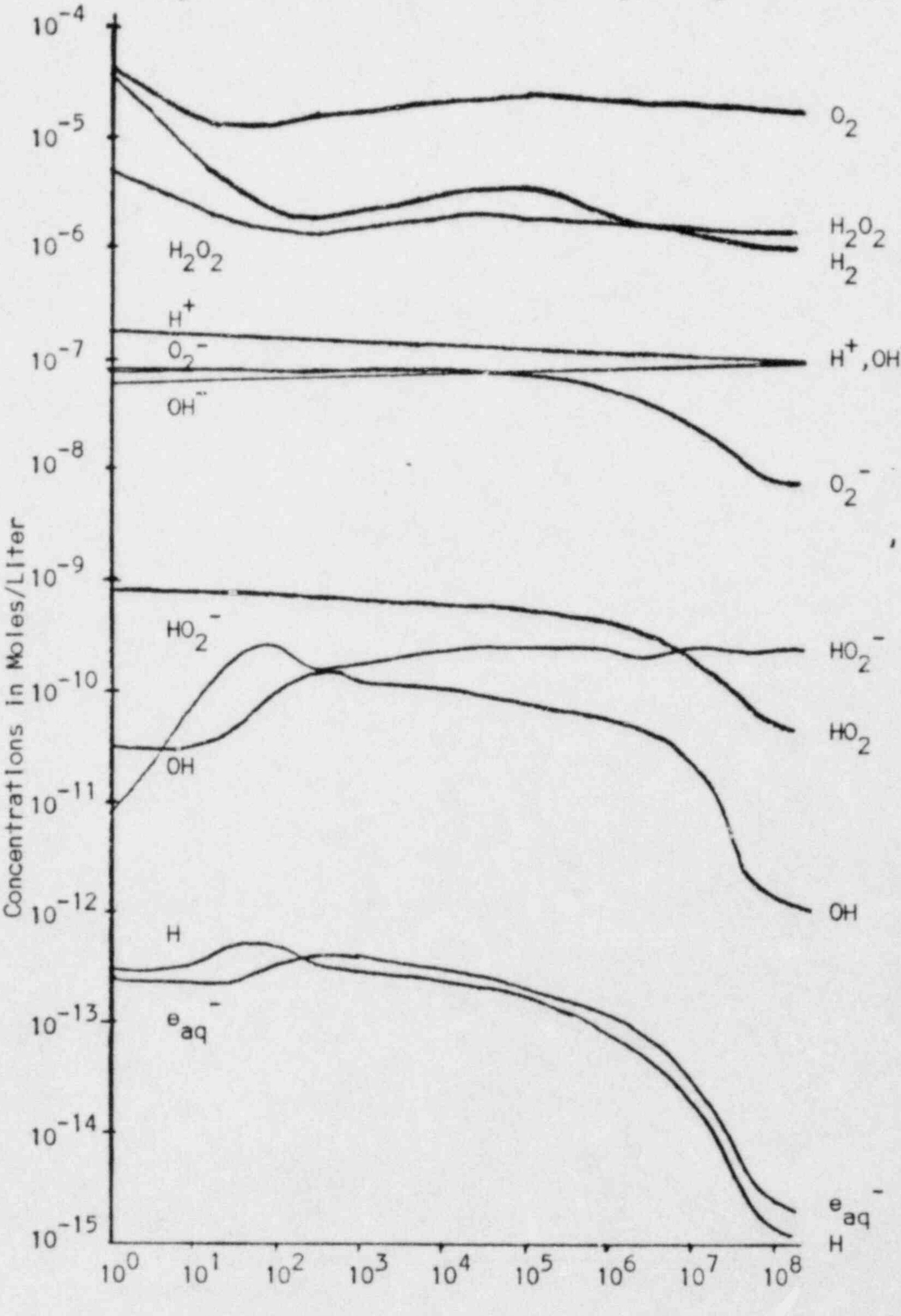


Figure XXIII

Time Dependent Concentrations of Radiolytically Induced Species (at 100°C)



- Reduction of OH radical via oxidation of M^-

$$\begin{array}{l} OH + e^- = OH^- \\ \quad\; M^- = M + e^- \\ \hline OH + M^- = OH^- + M \end{array} \qquad (4.28)$$

- Oxidation of H radical via reduction of M

$$\begin{array}{l} \quad\; H = H^+ + e^- \\ e^- + M = M^- \\ \hline H + M = H^+ + M^- \end{array} \qquad (4.29)$$

- Capture of e_{aq}^- via reduction with M

$$e_{aq}^- + M \rightarrow M^- + (H_2O) \qquad (4.30)$$

In view of the fact that the recombination reactions in general lead to chain reactions converting H_2 and O_2 back to water, the potential impact of these impurities is to break up the chain reactions by replacing H, OH with H^+ and OH^-. (Similar effects are possible for metallic impurities such as Fe.+2)

To understand the quantitative impacts of impurities, it is necessary to utilize a model developed by Jenks and Greiss (Reference 30) for the case of excess dissolved H_2 and O_2. Jenks and Greiss demonstrated that for the case where radiolysis/recombination is occurring in water with excess dissolved H_2 and O_2, the following standard reactions are heavily favored:

(7) $e^{-} + O_2 \xrightarrow{k_7'} HO_2 + OH^-$

(18) $OH + H_2 \xrightarrow{k_{18}} H + (H_2O)$

(21) $H + O_2 \xrightarrow{k_{21}} HO_2$

(25) $2HO_2 \xrightarrow{k_{25}} H_2O_2 + O_2$

(32) $HO_2 + H_2O_2 \xrightarrow{k_{32}} OH + O_2 + (H_2O)$

The main effects of impurities are summarized by the following oxidation/reduction reactions:

(33i) $M_i^{+n} + H \xrightarrow{k_{33i}} M_i^{+(n-1)} + H^+$

(34i) $M_i^{+n} + e^- \xrightarrow{k_{34i}} M_i^{+(n-1)} + (H_2O)$

(35i) $M_i^{+(n-1)} + OH \xrightarrow{k_{35i}} M_i^{+n} + OH^-$

- where M_i denotes any one of several species of impurities.

When chemical equilibrium is achieved, the following rate equations describe the equilibrium concentrations:

$$0 = \frac{d}{dt}[M_i^{+(n-1)}] = k_{33i}[H]_{eq}[M_i^{+n}]_{eq} + k_{34i}[e_{aq}^-]_{eq}[M_i^{+n}]_{eq} - k_{35i}[OH]_{eq}[M_i^{+(n-1)}]_{eq} \tag{4.31}$$

$$0 = \frac{d}{dt}[HO_2] = k_7'[e_{aq}^-]_{eq}[O_2]_{eq} + k_{21}[H]_{eq}[O_2]_{eq} - 2k_{25}[HO_2]_{eq}^2 - k_{32}[HO_2]_{eq}[H_2O_2]_{eq} \tag{4.32}$$

$$0 = \frac{d}{dt}[H_2O_2] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_{H_2O_2} - k_{32}[HO_2]_{eq}[H_2O_2]_{eq} + k_{25}[HO_2]^2_{eq} \qquad (4.33)$$

$$0 = \frac{d}{dt}[OH] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_{OH} + k_{32}[HO_2]_{eq}[H_2O_2]_{eq} - k_{18}[OH]_{eq}[H_2]_{eq} - k_{35_i}[OH]_{eq}[M_i^{+(n-1)}]_{eq} \qquad (4.34)$$

$$0 = \frac{d}{dt}[H] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_H + k_{18}[OH]_{eq}[H_2]_{eq} - k_{21}[H]_{eq}[O_2]_{eq} - k_{33_i}[H]_{eq}[M_i^{+n}]_{eq} \qquad (4.35)$$

$$0 = \frac{d}{dt}[e_{aq}^-] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_{e_{aq}^-} - k_7'[e_{aq}^-]_{eq}[O_2]_{eq} - k_{34_i}[e_{aq}^-]_{eq}[M_i^{+n}]_{eq} \qquad (4.36)$$

To algebraically solve this system of equations, Jenks and Greiss noted that there is only one reaction converting the excess H_2 back to water, namely:

$$OH + H_2 \xrightarrow{k_{18}} H + (H_2O)$$

Defining the rate of H_2O production via H_2 conversion as "R_R", the rate of oxidation of M_i may be expressed:

$$k_{35_i}[OH]_{eq}[M_i^{+(n-1)}]_{eq} = \frac{k_{35_i}[M_i^{+(n-1)}]_{eq} R_R}{k_{18}[H_2]_{eq}} \qquad (4.37)$$

Adding the equations defining the equilibrium concentrations of HO_2 and H_2O_2 yields the following:

$$2k_{32}[HO_2]_{eq}[H_2O_2]_{eq} = \frac{P_0 E_{\beta\gamma}(t)}{A_0 V_{core}} G_{H_2O_2} - k_{25}[HO_2]_{eq}^2 + k_7'[e_{aq}^-]_{eq}[O_2]_{eq} + k_{21}[H]_{eq}[O_2]_{eq} \qquad (4.38)$$

Subtracting the equations defining the equilibrium concentrations of HO_2 and H_2O_2 yields an expression for k_{25} $[HO_2]eq^2$

$$k_{25}[HO_2]_{eq}^2 = \frac{k_7'}{3}[e_{aq}^-]_{eq}[O_2]_{eq} + \frac{k_{21}}{3}[H]_{eq}[O_2]_{eq} - \frac{P_0 E_{\beta,\gamma}(t)}{A_0 V_{core}} G_{H_2O_2} \qquad (4.39)$$

This expression may be substituted into Equation 4.38 yielding:

$$k_{32}[HO_2]_{eq}[H_2O_2]_{eq} = \frac{2}{3}\frac{P_0 E_{\beta\gamma}(t)}{A_0 V_{core}} G_{H_2O_2} + \frac{k_7'}{3}[e_{aq}^-]_{eq}[O_2]_{eq} + \frac{k_{21}}{3}[H]_{eq}[O_2]_{eq} \qquad (4.40)$$

Utilizing this expression for the rate of reaction of HO_2 with H_2O_2 in the equation defining [OH]eq yields the following.

$$0 = \frac{d}{dt}[OH] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} \left(G_{OH} + \tfrac{2}{3} G_{H_2O_2}\right) + \frac{k_7'}{3}[e_{aq}^-]_{eq}[O_2]_{eq}$$

$$+ \frac{k_{21}}{3}[H]_{eq}[O_2]_{eq} - k_{18}[OH]_{eq}[H_2]_{eq}$$

$$- k_{35_i}[OH]_{eq}[M_i^{+(n-1)}]_{eq} \qquad (4.41)$$

Now substituting in:

$$R_R = k_{18}[OH]_{eq}[H_2]_{eq}$$

$$k_{35_i}[OH]_{eq}[M_i^{+(n-1)}]_{eq} = \frac{k_{35_i}[M_i^{+(n-1)}]_{eq} R_R}{k_{18}[H_2]_{eq}}$$

– the following can be obtained:

$$0 = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} (3G_{OH} + 2G_{H_2O_2}) + k_7'[e_{aq}^-]_{eq}[O_2]_{eq}$$

$$+ k_{21}[H]_{eq}[O_2]_{eq} - 3R_R\left(1 + \frac{k_{35_i}[M_i^{+(n-1)}]_{eq}}{k_{18}[H_2]_{eq}}\right) \qquad (4.42)$$

To obtain a complete solution of this equation, equations must be obtained for e_{aq}^- and H, specifically:

- $k_7'[e_{aq}^-]_{eq}[O_2]_{eq}$
- $k_{21}[H]_{eq}[O_2]_{eq}$

The equation defining equilibrium H concentration may be expressed:

$$0 = \frac{d}{dt}[H] = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_H + R_R - k_{21}[H]_{eq}[O_2]_{eq}$$

$$- k_{33_i}[H]_{eq}[M_i^{+n}]_{eq} \qquad (4.43)$$

Solving for k_{21} $[H]_{eq}[O_2]_{eq}$ yields:

$$k_{21}[H]_{eq}[O_2]_{eq} = \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} G_H + R_R - k_{33_i}[H]_{eq}[M_i^{+n}]_{eq} \tag{4.44}$$

Using the equation defining equilibrium e_{aq}^- concentrations, an expression can be obtained for k_7' $[e_{aq}^-]$eq $[O_2]$eq:

$$k_7'[e_{aq}^-]_{eq}[O_2]_{eq} = \frac{P_o E_{\beta\gamma}(t)}{A_o V_{core}} G_{e_{aq}^-} - k_{34_i}[e_{aq}^-]_{eq}[M_i^{+n}]_{eq} \tag{4.45}$$

Substituting these expressions (Equations 4.42, 4.43) into Equation 4.40 yields:

$$\begin{aligned} 0 = {} & \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} (3G_{OH} + 2G_{H_2O_2} + G_{e_{aq}^-} + G_H) \\ & - k_{33_i}[H]_{eq}[M_i^{+n}]_{eq} - k_{34_i}[e_{aq}^-]_{eq}[M_i^{+n}]_{eq} \\ & - R_R \left(2 + \frac{3k_{35_i}[M_i^{+(n-1)}]_{eq}}{k_{18}[H_2]_{eq}}\right) \end{aligned} \tag{4.46}$$

Subtracting the equation defining Equilibrium $M_i^{+(n-1)}$ concentration from this expression yields:

$$\begin{aligned} 0 = {} & \frac{P_o E_{\beta,\gamma}(t)}{A_o V_{core}} (3G_{OH} + 2G_{H_2O_2} + G_{e_{aq}^-} + G_H) \\ & + k_{35_i}[OH]_{eq}[M_i^{+(n-1)}]_{eq} - R_R \left(2 + \frac{3k_{35_i}[M_i^{+(n-1)}]_{eq}}{k_{18}[H_2]_{eq}}\right) \end{aligned} \tag{4.47}$$

Noting that:

$$k_{35_i}[OH]_{eq}[M_i^{+(n-1)}]_{eq} = \frac{k_{35_i}[M_i^{+(n-1)}]_{eq}}{k_{18}[H_2]_{eq}} R_R$$

An expression for the net recombination rate can now be defined:

$$R_R = \frac{P_o E_{\beta\gamma}(t)}{A_o V_{core}} \cdot \frac{3G_{OH} + 2G_{H_2O_2} + G_{e_{aq}^-} + G_H}{2 + \dfrac{k_{35_i}[M_i^{+(n-1)}]_{eq}}{k_{18}[H_2]_{eq}}} \tag{4.48}$$

This equation may be directly compared to the net rate of decomposition of H_2O based on G_{-H_2O}, defined as:

$$R_D = \frac{PoE^{(t)}_{\beta,\gamma}}{A_0 V_{core}} G_{-H_2O} \tag{4.49}$$

By definition, if it is assumed that chemical equilibrium exists and:

$$2H_2O \overset{\beta,\ \gamma}{\rightleftharpoons} 2H_2 + O_2 \tag{4.50}$$

- then the net rate of recombination must equal the net rate of decomposition for the existing dose intensity. This allows the direct computation of an upper limit on the impurity levels in water where radiolytic stability is assured for a given dissolved level of H_2 gas. To define this limit, it is noted that equilibrium breaks down when:

$$R_D \geq R_R \tag{4.51}$$

Substituting in for R_D and R_R and then simplifying yields the following relationship for the breakdown of equilibrium.

$$\sum_i k_{35_i} [M_i^{+(n-1)}]_{eq} \geq k_{18} [H_2]_{eq} \left(\frac{3}{4} G_{OH} + \frac{1}{2} G_{H_2O_2} + \frac{1}{4} G_{e_{aq}} + \frac{1}{4} G_H - \frac{1}{2} G_{-H_2O}\right) \tag{4.52}$$

Substituting in for the G values from Figure V, it is noted that:

$G_{OH} = 2.34$

$G_{H_2O_2} = 0.70$

$G_{eaq-} = 2.31$

$G_H = 0.55$

$G_{-H_2O} = 3.74$ (Reference 5)

Hence:

$$\sum_i k_{35_i} [M_i^{+(n-1)}]_{eq} \geq 0.95 k_{18} [H_2]_{eq} \qquad (4.53)$$

It is now necessary to evaluate the specific types of impurities (M_i) present and how effectively they react with OH radicals. There are basically three types of impurities likely to be present in the coolant water following an accident.

- <u>Suspended solids related to the damaged cladding</u>

  Gordon, Schmidt, and Honekamp in Reference 22 noted that while zirconium oxide or hydroxide may become suspended in the water after an accident where an extensive Zr-H_2O reaction has taken place, the zirconium ions tend to hydrolyze very easily via the equilibrium reaction:

$$Zr(OH)_4 + H^+ \rightleftharpoons Zr(OH)_3^+ + H_2O \qquad (4.54)$$

$K_a = 7 \times 10^{-2}$

(In range of pH $\cong$ 6, the ratio $Zr(OH)_3^+/Zr(OH)_4 = 1.4 \times 10^{-5}$.) Because of the very low solubility product of $Zr(OH)_4$ ($K_{sp} = 1.1 \times 10^{-54}$), the amount of Zr in solution as hydroxide or ion would be negligible.

- Fission product impurities

These species in the reactor coolant are the result of fuel damage caused by prolonged inadequate core cooling. Large concentrations of these types of impurities in coolant water can only occur if substantial overheating of the clad (and hence generation of excess H_2 from the $Zr-H_2O$ reaction) has already occurred. These impurity effects are discussed in Section 4.3.1.

- Chemical impurities not related to fuel damage

A number of trace metallic and halide type impurities can also be present in the coolant water. In this regard, it must be noted that the operation of the Reactor Water Cleanup System may be precluded due to excessive activity in the coolant. Hence, metallic impurities will be limited to the levels existing in the core at the start of the accident. These types of impurities are discussed in Section 4.3.2.

4.3.1 Fission Product Impurities

While the activities present in reactor coolant following severe damage to the fuel may be appreciably large from a radiological point of view, a majority are relatively small from a chemistry point of view. A good example of this is an analysis of the molar concentrations of fission products present in the reactor coolant following the TMI-2 accident. Reference 23 provided a summary of the results of various chemistry samples analyzed by Bettis Atomic Power Laboratory, Oak Ridge National Laboratory, and Savannah River Laboratory following the TMI-2 accident. The measured activities (in μC/ml) can be converted to molar concentrations via the following equation.

$$[X](\text{moles/liter}) = \frac{A_x(\mu C/\text{ml})(10^{-3})(3.7 \times 10^{10}/C \cdot \text{sec})}{\lambda_X(\text{sec}^{-1})(6.023 \times 10^{23}/\text{mole})} \tag{4.55}$$

Utilizing this expression, the table in Figure XXIV was prepared using the highest activity values measured. In reviewing the results of these calculations, it is noted that the only fission product isotopes of significance from a chemistry point of view are: Cs^{137}, Sr^{90}, I^{131}, I^{133} which upon combining I^{131} and I^{133} all have concentrations greater than 9.0 x 10^{-7} moles/liter. All other fission product species exist in concentrations far too rarefied to have any significant impact on the recombination reactions. With regard to using TMI-2

FIGURE XXIV

COMPARISON OF ISOTOPE ACTIVITIES AND CONCENTRATIONS IN THE TMI-2 REACTOR COOLANT

Radioisotope X	Half-life $t_{1/2}$ (sec.)	Decay Constant λ_X (sec^{-1})	Activity A_X ($\frac{\mu C}{ml}$)	Data Source	Radioisotope Concentration $[X]$ ($\frac{moles}{liter}$)
I^{131}	6.912×10^{5}	1.00281×10^{-6}	1.4×10^{4}	Bettis	8.576×10^{-7}
I^{133}	7.488×10^{4}	9.25677×10^{-6}	6.8×10^{3}	Bettis	4.513×10^{-8}
Cs^{134}	6.307×10^{7}	1.09897×10^{-8}	6.3×10^{1}	Bettis	3.522×10^{-7}
Cs^{136}	1.123×10^{6}	6.17118×10^{-7}	1.8×10^{2}	Bettis	1.792×10^{-8}
Cs^{137}	9.461×10^{8}	7.32651×10^{-10}	2.7×10^{2}	Bettis	2.264×10^{-5}
Sr^{89}	4.32×10^{6}	1.6045×10^{-7}	5.4×10^{0}	Bettis	2.067×10^{-9}
Sr^{90}	9.145×10^{8}	7.57915×10^{-10}	5.0×10^{1}	ORNL	4.053×10^{-6}
Ru^{106}	3.179×10^{7}	2.18003×10^{-8}	3.6×10^{1}	Bettis	1.014×10^{-7}
Ba^{140}	1.106×10^{6}	6.2676×10^{-7}	2.1×10^{1}	Bettis	2.058×10^{-9}
Ba^{136} (m)	3.5×10^{-1}	1.98042×10^{0}	9.0×10^{1}	SRL	2.792×10^{-15}
La^{140}	1.44×10^{5}	4.81352×10^{-6}	1.6×10^{2}	ORNL	2.042×10^{-9}
Mo^{99}	2.376×10^{5}	2.91728×10^{-6}	1.8×10^{2}	ORNL	3.790×10^{-9}
Te^{132}	2.808×10^{5}	2.46847×10^{-6}	2.0×10^{2}	Bettis	4.977×10^{-9}
Ce^{141}	2.765×10^{6}	2.50704×10^{-7}	1.05×10^{2}	SRL	2.573×10^{-8}

post-accident chemistry samples for analysis of radiolysis at Millstone Unit I, it should be noted that the TMI-2 accident is clearly an accident beyond the normal design bases of the plant. Hence, use of TMI-2 fission product impurities represents a significant level of conservatism over normal DBA conditions at Millstone Unit I in spite of the differences in core power ratings and total anticipated liquid inventories.

To define the types of ionic species likely present in the coolant water, the results of a review of post accident fission product chemistry carried out in Reference 31 was utilized. Based on Reference 31, it may be concluded that the following molecules and ionic species are the most likely to be found.

- <u>Cesium (Isotopes: Cs^{137}, Cs^{134})</u>

$CsI \rightarrow Cs^+ + I^-$

$CsOH$ (insoluble)

Cs^+ is predominant

o Strontium (Predominantly: Sr^{90})

SrI_2 (not as chemically stable as CsI) $\rightarrow Sr^+ + 2I^-$

$Sr(OH)_2 \rightarrow Sr(OH)^+ + OH^-$ (possible)

Sr^{+2} is predominant

o Iodine (Isotopes: I^{131}, I^{133})

I_2^-

$HI \rightarrow H^+ + I^-$

I_3

I

I^-

CH_3I

IO_3

HOI

HOI^- (not chemically stable)

I^- is dominant

With regard to the types of oxidation/reduction reactions capable of causing a breakdown in equilibrium, the following is noted.

o Reactions involving Cs

The only potential Cs reaction which could scavenge OH radicals is:

$$Cs^+ + OH \rightarrow Cs^{+2} + OH^-$$

-however as with all other alkali metals (e.g.: sodium, lithium, potassium, etc.) the rate constant is so small it is not possible to experimentally measure. Hence Cs^+ ions pose no real threat to breaking down the natural recombination processes.

- Reactions involving Sr

The only potential Sr reaction which would scavenge OH radicals is:

$$Sr^{+2} + OH \longrightarrow Sr^{+3} + OH^-$$

Again, the rate constant of this is too small to be experimentally measured, hence Sr^{+2} ions pose no threat to breaking down the natural recombination reactions.

- Reactions involving I

The net scavenging reaction is: $I^- + OH \longrightarrow I + OH^-$, via:

$$I^- + OH \longrightarrow HOI^- \xrightarrow[(fast)]{} OH^- + I$$

can have an effect if the I^- concentration is excessively large. The measured rate constant is: $k_{I^-} = 1.2 \times 10^{10}$ based on Reference 19. In reviewing the results of the TMI-2 post-accident chemistry sample, however, where total iodine concentrations was on the order of 3.2×10^{-6} moles/liter*, if it were assumed that all iodine were in the form of I^- ions, the product $k_{I^-}\left[I^-\right]eq$ is still less than of $0.95k_{18}\left[H_2\right]eq$, when $\left[H_2\right]eq$ is computed for the postulated range of TMI-2 accident f_{Zr-H_2O} values. The key item to be recalled is that the excessively large values of dissolved I^- can only occur from extensive fuel damage and hence large f_{Zr-H_2O} values (which yield correspondingly large $\left[H_2\right]eq$ values.)

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*This value was obtained by correcting for stable, and long-lived radioactive iodine isotopes (I^{127}; I^{129}) using results from the ORIGEN Code.

On the other end of the accident spectrum where: $f_{Zr-H_2O} = 0.0$, dissolved H_2 concentrations will be 7.9×10^{-6} moles/liter (note: Figure IX on page 45). Assuming severe iodine spiking as a result of a transient of roughly 50 μC/ml or 1.15×10^{-8} moles/liter, $0.95k_{18} [H_2]eq$ is 2.44 times greater than $k_{I^-}[I^-]eq$. Hence net recombination would still be predicted.

The same is true for iodate ions (IO_3^-). Based on equilibriation calculations in Reference 31 at 25°C, $[I^-]eq >> [IO_3^-]eq$ by several orders of magnitude. Furthermore, the measured rate constant (Reference 19) is roughly 5×10^7 in the pH range of interest.

Because of this iodate ions also pose no real threat to breaking down the natural recombination processes.

In view of these considerations of the fission product impurities in chemically appreciable concentrations, only the iodide ion species are of significance to the question of radiolysis and recombination. The chief mechanism which prevents these species from breaking down the natural recombination tendency is the fact that their existence in significant concentrations can only occur along with substantial H_2 generation. This concern is clearly self-limiting in nature. Of greater concern would be the impurities which are not related to fuel damage and whose existence is independent of the extent of the metal water reaction. These are discussed in the following section.

4.3.2 Chemical Impurities Not Related to Fuel Damage

As noted in Section 4.3, a third potential source of impurities capable of disrupting the normal recombination process are impurities not related to the damage of reactor fuel. These include halide impurities (predominantly Cl^-) beyond the capability of the water purification systems and the matallic type impurities normally formed as a result of "crud" buildup.

In accordance with Tech, Spec. 3.6.C.4 the feedwater quality at Millstone Unit 1 is maintained to chloride levels of less than .5 ppm via water treatment*. These chloride concentrations correspond to a molar concentration of $[CI^-] = 1.4 \times 10^{-5}$ moles/liter. Deviations from this limit requires a plant shutdown. Additionally, the potential of this level of Cl^- interferring with recombination is further diminished by noting that the rate constant of the reaction:

$$OH + Cl^- \longrightarrow ClOH^-$$

is less than 1×10^6 (Reference 19) and the rate constant for reaction with H is less than 1×10^5 (Reference 18). Because of these considerations, chloride ions have an insignificant potential for disrupting recombination.

Metallic ion impurities are another potential source for scavenging OH and H radicals.

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*Nominal chloride levels are in the range of 20 ppb, $[Cl^-] = 5.6 \times 10^{-7}$ moles/liter.

To obtain a conservative estimate of the particular species and concentrations of soluble impurities the results of a detailed chemistry sampling program at the Brunswick Unit 2 B.W.R. were utilized (Reference 32). The highest measured concentrations are summarized in the table in Figure XXV. In Appendix K of Volume II analysis is performed to define the predominant ionic forms of the impurities. This review concludes that assuming the +2 oxidation state for the impurities is sufficiently conservative. As noted in the table, various insoluble iron oxides are the predominant impurity species by several orders of magnitude, but the soluble iron (assumed to be mainly Fe^{+2}) is only in the ppb range. There are several effects which can alter levels of impurities.

- severe reactor transients were determined to cause a 475% increase in soluble iron. (Reference 32).
- decreasing water temperature is known to increase solubility of certain impurities.
- operation of the Low Pressure ECCS systems will provide dilution effect from water not normally exposed to the impurities coming from the feedwater and condensate systems. (Note that the torus liquid volume is roughly 10.4 times the anticipated core liquid volume.)

FIGURE XXV

METALLIC CORROSION PRODUCT IMPURITIES

Metallic (Impurity)	Insoluble Species Concentration (ppb)	Soluble Species Concentration (ppb)	Soluble Species Molar Concentration (moles/liter)
Fe	520	6.9	1.236×10^{-7}
Zn	0.64	0.69	1.055×10^{-8}
Cu	4.1	17.0	2.676×10^{-7}
Co	0.34	0.28	4.75×10^{-9}
Mn	0.32	1.4	2.55×10^{-8}
Ni	30.0	12.0	2.044×10^{-7}

Based on a review of the reaction rates of these impurities with OH radical the following may be noted:

- $Fe^{+2} + OH \longrightarrow Fe^{+3} + OH^-$ $k = 3.4 \times 10^8$
- $Cu^{+2} + OH \longrightarrow Cu^{+3} + OH^-$ $k = 3.5 \times 10^8$
- $Co^{+2} + OH \longrightarrow Co^{+3} + OH^-$ $k = 2.0 \times 10^6$
- $Ni^{+2} + OH \longrightarrow Ni^{+3} + OH^-$ $k = 5.0 \times 10^5$
- $Zn^{+2} + OH \longrightarrow Zn^{+3} + OH^-$ $k = 5.0 \times 10^5$
- $Mn^{+2} + OH \longrightarrow Mn^{+3} + OH^-$ $k = 1.4 \times 10^8$

By considering the reaction rates and the relative molar concentrations of impurities it may be concluded that only Fe, Cu, and Mn impurities are of significance to the question of radiolysis and recombination. To provide sufficient conservatism in the analysis to bound possible abnormal impurity concentrations the maximum impurity levels below (Reference 36) are assumed. These values are substantially above the worst case observed levels of metallic impurities based on data provided by General Electric Company, (e.g., they include data from reactor startups when such impurities are at maximum values).

- $[Fe^{+2}] = 32.775$ ppb $= 5.871 \times 10^{-7}$ moles/liter
- $[Cu^{+2}] = 30$ ppb $= 4.722 \times 10^{-7}$ moles/liter
- $[Mn^{+2}] = 25$ ppb $= 4.554 \times 10^{-7}$ moles/liter

Again utilizing the stability criteria defined in Equation 4.53, spontaneous natural recombination can only breakdown when:

$$\sum_{i} k_{35_i} [M_i^{+(n-1)}]_{eq} \geq 0.95\, k_{18} [H_2]_{eq} \qquad (4.56)$$

Upon making substitutions for the impurity reactions:

$$\sum_i k_{35_i}[M_i^{+(n-1)}]_{eq} = k_{Fe^{+2}}\,[Fe^{+2}]_{eq} + k_{Cu^{+2}}\,[Cu^{+2}]_{eq} + k_{Mn^{+2}}[Mn^{+2}]$$

$$= 428.64 \tag{4.57}$$

Whereas: at T = 25°C (where k_{18} is at a minimal value) the potential values of the recombination term are as follows when ε_{H_2O} = 110 lbs.:

f_{Zr-H_2O}	$[H_2](f_{Zr-H_2O})$ (in moles/liter)	$0.95k_{18}[H_2]$
0.00	7.92×10^{-6}	338.58
1×10^{-3}	9.75×10^{-6}	416.81
2×10^{-3}	1.16×10^{-5}	495.90
5×10^{-3}	1.71×10^{-5}	731.03
6.12×10^{-3}	1.92×10^{-5}	820.80
1×10^{-2}	2.63×10^{-5}	1124.33
5×10^{-2}	9.98×10^{-5}	4266.45
1×10^{-1}	1.92×10^{-4}	8208.00
2×10^{-1}	3.75×10^{-4}	16031.25
5×10^{-1}	9.27×10^{-4}	39629.25

If it were assumed that less boiling phase radiolysis had occurred (e.g., ε_{H_2O} = 14 lbs) the following would be obtaind:

f_{Zr-H_2O}	$[H_2](f_{Zr-H_2O})$ (in moles/liter)	$0.95k_{18}[H_2]$
0.00	1.62×10^{-6}	69.26
1×10^{-3}	3.46×10^{-6}	147.92
2×10^{-3}	5.3×10^{-6}	226.58
5×10^{-3}	1.08×10^{-5}	461.70
6.12×10^{-3}	1.29×10^{-5}	855.00
1×10^{-2}	2.0×10^{-5}	3997.13
5×10^{-2}	9.35×10^{-5}	7908.75
1×10^{-1}	1.85×10^{-4}	15774.75
2×10^{-1}	3.69×10^{-4}	39330.00

In either case, it is important to note the following:

- For the metal-water reaction requiring minimal amount of radiolytic decomposition to reach the flammability ($f_{Zr-H_2O} = 6.12 \times 10^{-3}$), the reactor coolant is <u>stable</u> against any further radiolytic decomposition at the time boiling ceases.

- For accidents yielding greater metal-water reactions than $f_{Zr-H_2O} = 6.12 \times 10^{-3}$, the reactor coolant is even <u>more stable</u> against further radiolytic decomposition.

- For accidents in which the extent of the metal-water reaction is very small (generally less than $f_{Zr-H_2O} = .002$) there will be additional net radiolysis until the dissolved H_2 level in the coolant builds up to a level where equilibrium between radiolytic decomposition and recombination is achieved. (It should be pointed out that these accident scenarios correspond to the best estimate for normal ECCS response to design basis LOCA, e.g., $f_{Zr-H_2O} \leq .002$).

The pertinent questions to be asked at this point are:

- How much net radiolysis will have to occur to assure equilibrium?

- What are the impact of this on the flammability limit margins in containment?

To addressing the first question the stable level of H_2 is given by solving for $[H_2]$ in Equation 4.53:

$$[H_2]_{eq} \geq \frac{\sum_i k_{35_i} [M_i^{+(n-1)}]_{eq}}{0.95\ k_{18}} \cong 1.003\times10^{-5} \text{ moles/liter} \tag{4.58}$$

By utilizing Equation 3.26 it is possible to solve for ε_{H_2O} (the extent of net radiolysis) in terms of the magnitude of f_{Zr-H_2O}. If:

$$[H_2]_{eq} = 1.003\times10^{-5} \text{ moles/liter}$$

$$= \frac{1}{V_{liq}}\left(\frac{1}{\gamma_{H_2}+1}\right)[n_{H_2} + 2 f_{Zr-H_2O} n_{Zr} + \varepsilon_{H_2O} X_{H_2}] \tag{4.59}$$

Then:

$$\varepsilon_{H_2O} = \frac{(\gamma_{H_2}+1)[H_2]_{eq} V_{liq.} - n_{H_2} - 2 f_{Zr-H_2O} n_{Zr}}{X_{H_2}} \tag{4.60}$$

Substituting in values yields the following expression:

$$\varepsilon_{H_2O} = 141.738 \text{ lbs.} - (2.8034\times10^4) f_{Zr-H_2O} \tag{4.61}$$

To address the question of the impacts of this additional net radiolysis on containment flammability of the table in Figure III may be consulted. This table summarizes the amount radiolytic decomposition necessary to achieve flammability for a given extent of metal-water reaction. Taking into account sensitivities and uncertainties, it is still important to note that: <u>two to three times the values</u> defined in Equation 4.61 are necessary in order to barely reach flammability.

The significant of this analysis is as follows:

- When worst case metallic corrsion product impurities are assumed the radiolytic decomposition is either stabilized as a result of the metal-water reaction or by the net radiolysis necessary to achieve dissolved H_2 concentrations defined in Equation 4.58.

- In either case the H_2, O_2 containment gas concentrations are below the limits of flammability.

CHAPTER 5

THE NEED FOR ADDITIONAL COMBUSTIBLE GAS CONTROL FEATURES

5.0 EFFECTIVENESS OF INERTING

The analyses carried out in this report has shown that if the containment is pre-inerted with excess N_2, such that initial O_2 concentrations are at or below 4% then:

- there is no metal-water reaction envisioned which can yield flammability.

- large metal-water reactions add excess H_2 to the containment which is actually <u>beneficial</u> for two reasons:

  (a) it acts as a diluent for O_2 gas which is the critical limitation in avoiding flammability.

  (b) it promotes the stabilization of the radiolytic decomposition and recombination process and allows one to cope with large impurity concentrations in the water.

- very small metal-water reactions will result in net radiolysis that adds excess H_2 to the extent that further radiolysis is stabilized for the existing impurity concentration present. The H_2 and O_2 gases added were shown to be insufficient to yield flammable mixtures even when maximum possible impurity levels were assumed.

The most desireable feature of inerting is that it amounts to a passive combustible gas control scheme requiring no additional mechanical or operator actions. This is important due to the fact that it permits the plant operators to focus attention on more critical safety functions such as:

- assuring long term decay heat removal.
- assuring logn term containment heat removal.
- assuring containment integrity.

By taking credit for N_2 inerting and the natural physical processes occurring when radiation interacts with water, it has been shown that there is no need to take credit for either containment purging or for post-accident N_2 pressurization, in order to assure combustible gas control.

5.1 EFFECTIVENESS OF BACKFITTING RECOMBINERS

This analysis has demonstrated that one of the key physical features for assuring combustible gas control is the existence in all cases of an H_2 gas overpressure in the containment. This H_2 gas overpressure assures a dissolved H_2 concentration in coolant liquids which is sufficient to stabilize radiolysis (but which is insufficient to become flammable). In assessing what a recombiner unit will do towards combustible gas control the following should be kept in mind:

- removal of the H_2 and O_2 gas from the containment gas via a recombiner system will reduce the overpressure that these gases exert on the coolant water.
- reduced H_2,O_2 gas overpressure decreases H_2 and O_2 gas solubility in the coolant water.
- reduced gas solubility implies that more H_2 and O_2 gas will leave the coolant water and enter the containment gas region, thus reducing dissolved gas concentrations in the coolant.
- if a substantial reduction in dissolved H_2 gas concentration occurs, net radiolysis and generation of more H_2 and O_2 gas will ensue in an attempt to restore the equilibrium balance.

In short: backfitting a recombiner system to an already inerted containment may achieve little. This is because it attempts to "fight" a physical process which desires to seek an equilibrium condition.

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Analysis of Post-Accident Combustible Gas Control at Millstone Unit I

Volume II

Supplemental Analyses
and
Computer Simulations

NOTICE

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VOLUME II

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APPENDIX A

CURVEFIT AND ERROR ANALYSIS OF H_2-O_2 FLAMMABILITY DATA

In order to facilitate the determination of the impacts of short term metal-water reactions and radiolysis on flammability within the containment simple curvefits were generated using the IBM 370 package for curvefitting and plotting: SKETCHIT (Reference 2).

Figure A-1 shows the input data for the upper region (where $[H_2]_{lim}$ varies as a function of $[O_2]_c$) and the error analysis. Figure A-2 shows the resultant fitted curve which is used throughout the analysis discussed in this report.

```
*A MILLSTONE 1 FLAMMABILITY LIMITS

    X-DESCRIPTION                               Y-DESCRIPTION
 % O  CONTENT            0.      20.946 % H  CONTENT              0          72.0

                                   -3

     A0              A1              A2              A3
-0.7119376D 02  0.2020868D 02 -0.1054300D 01  0.1990303D-01

     X               Y               Y CALC      Y-Y CALC      PCT DIF
      4.900000        6.000000        4.856573      1.143427     19.057
      5.000000        4.000000        5.979985     -1.979985     49.500
      5.049999        8.000000        6.536008      1.463992     18.300
      5.099999        7.000000        7.088280     -0.088280      1.261
      5.750000       12.000000       13.932065     -1.932065     16.101
      5.900000       16.000000       15.424889      0.575111      3.594
      7.299999       29.000000       27.888504      1.111496      3.833
     10.000000       45.500000       45.365936      0.134064      0.295
     12.549999       55.000000       55.711563     -0.711563      1.294
     16.599991       65.000000       64.789536      0.210464      0.324
     20.000000       71.000000       70.483780      0.516220      0.727
     20.945999       72.000000       72.442413     -0.442413      0.614

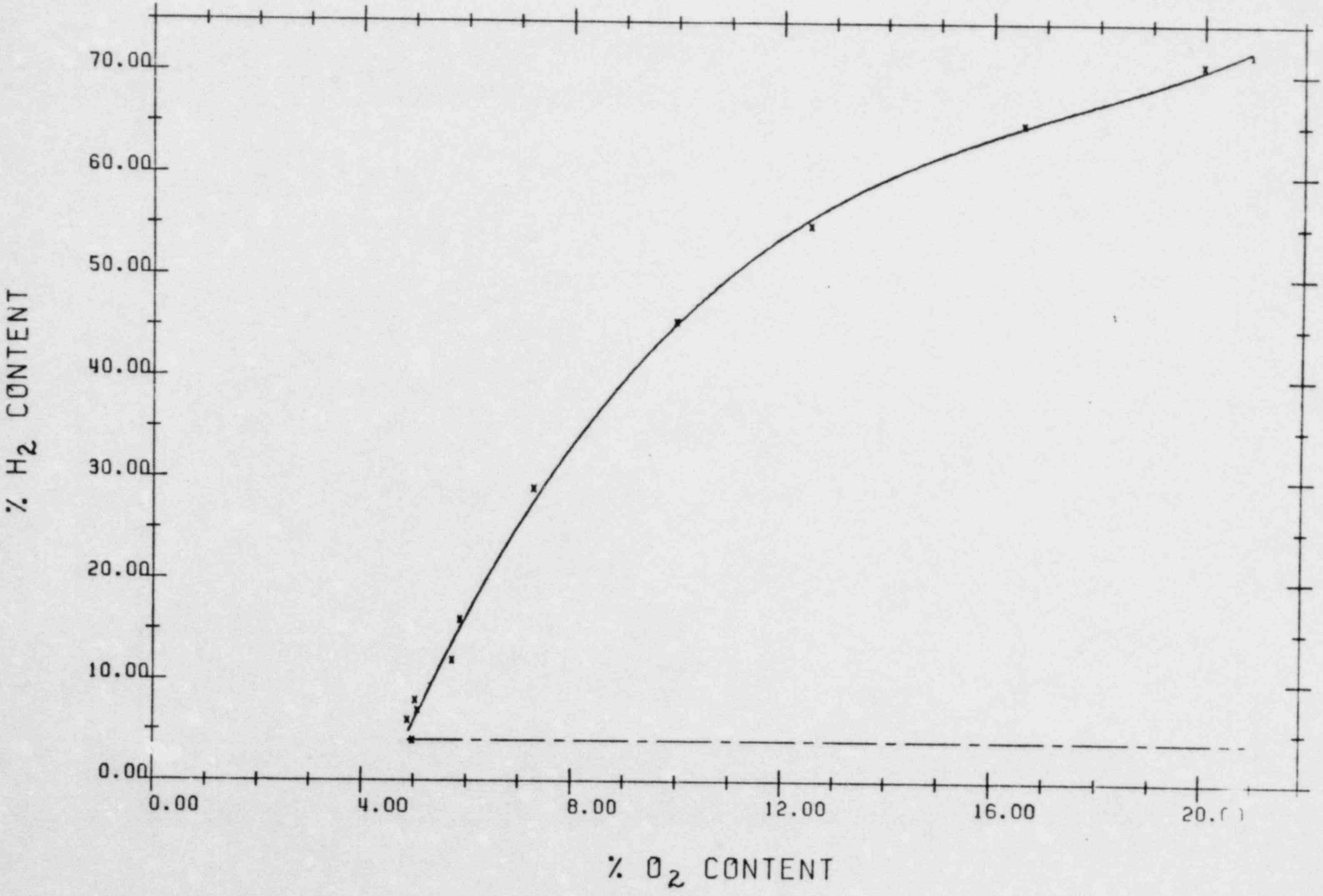
 RMS ERROR IS     1.068826


                                   -1

     A0              A1
 0.3999999D 01  0.4485491D-07

     X               Y               Y CALC      Y-Y CALC      PCT DIF
      5.000000        4.000000        3.999999      0.000001      0.000
     20.945999        4.000000        4.000000      0.0           0.0

 RMS ERROR IS     0.000001
```



MILLSTONE 1 FLAMMABILITY LIMITS

APPENDIX B

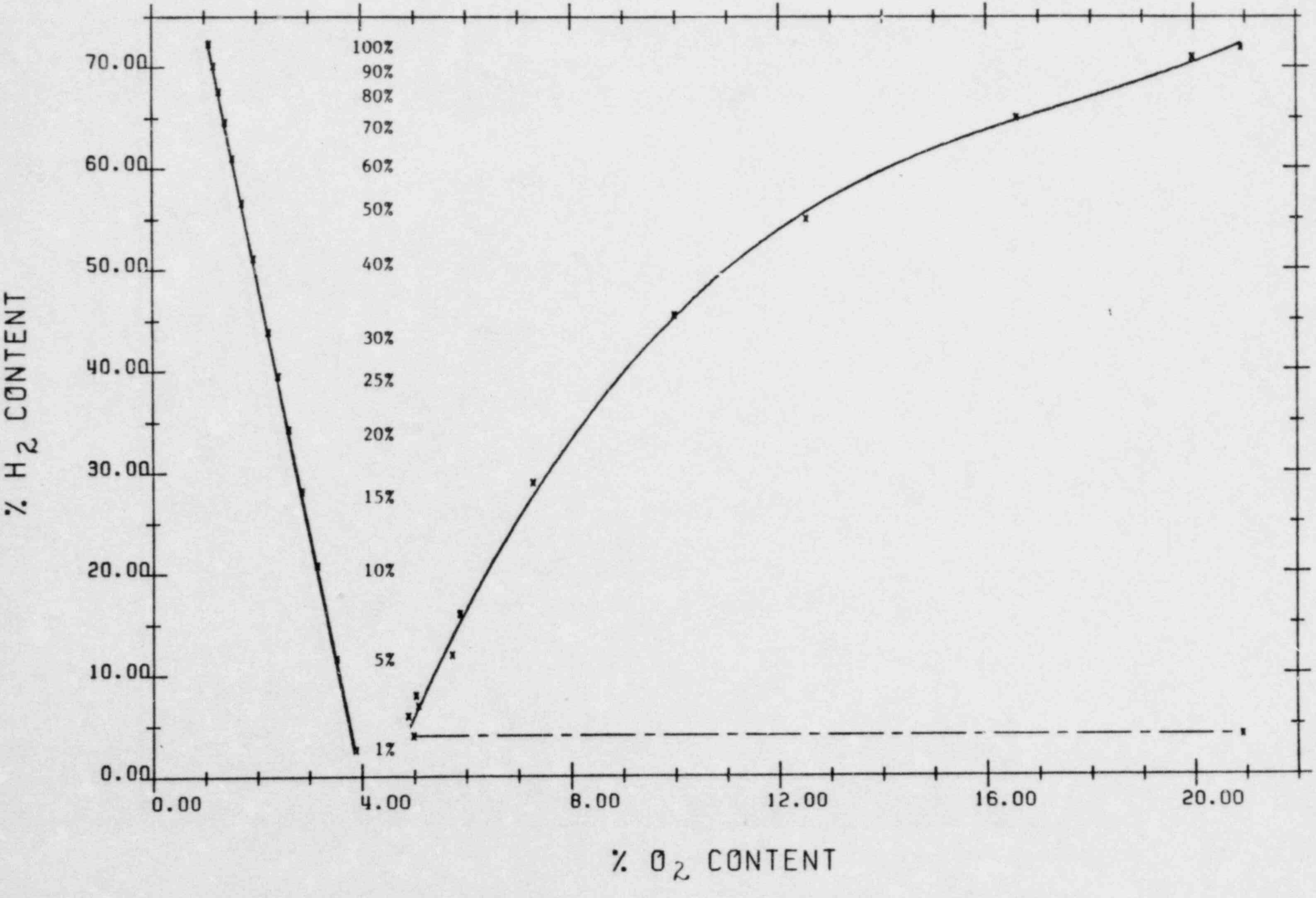
CALCULATION OF THE IMPACTS OF $Zr-H_2O$ REACTION ON CONTAINMENT GAS CONCENTRATIONS

In order to assess the impacts of the short term $Zr-H_2O$ reaction, a simple calculation was performed for varying values of f_{Zr-H_2O}. Figure B-1 is a listing of the computer program used to calculate $[O_2]_c$ and $[H_2]_c$ as a function of f_{Zr-H_2O} with all values expressed in %. Figure B-2 shows the results of this calculation which is plotted in Figure B-3.

```
FORTRAN IV G LEVEL  21                MAIN              DATE = 82130          09/51/03              PAGE 0001

                C
                C     CALCULATION OF ZIRC WATER REACTION
                C              JOHN BICKEL
                C
  0001                REAL * 8 X, Y, Z
  0002                DO 10 I=1,32
  0003                Z=DFLOAT(I)
  0004                IF(I.GE.15) Z=5.D0 * (Z-14.D0) + 10.D0
  0005                Y = (2.7085D2 + 2.D-2 * Z * 3.52916D5)/
                     A    (2.7085D5 + 2.D-2 * Z * 3.52916D5)
  0006                X =  1.0834D4 / (2.7085D5 + 2.D-2 * Z * 3.52916D5)
  0007                WRITE (6,20) Z, X, Y
  0008             20 FORMAT (3(5X,D10.3))
  0009             10 CONTINUE
  0010                STOP
  0011                END
```

f_{Zr-H_2O}	$[O_2]_c$	$[H_2]_c$
0.100D 01	0.390D-01	0.264D-01
0.200D 01	0.380D-01	0.505D-01
0.300D 01	0.371D-01	0.734D-01
0.400D 01	0.362D-01	0.953D-01
0.500D 01	0.354D-01	0.116D 00
0.600D 01	0.346D-01	0.136D 00
0.700D 01	0.339D-01	0.155D 00
0.800D 01	0.331D-01	0.173D 00
0.900D 01	0.324D-01	0.191D 00
0.100D 02	0.317D-01	0.208D 00
0.110D 02	0.311D-01	0.224D 00
0.120D 02	0.305D-01	0.239D 00
0.130D 02	0.299D-01	0.254D 00
0.140D 02	0.293D-01	0.268D 00
0.150D 02	0.285D-01	0.282D 00
0.200D 02	0.263D-01	0.343D 00
0.250D 02	0.242D-01	0.395D 00
0.300D 02	0.224D-01	0.439D 00
0.350D 02	0.209D-01	0.478D 00
0.400D 02	0.196D-01	0.511D 00
0.450D 02	0.184D-01	0.540D 00
0.500D 02	0.174D-01	0.566D 00
0.550D 02	0.164D-01	0.589D 00
0.600D 02	0.156D-01	0.610D 00
0.650D 02	0.148D-01	0.629D 00
0.700D 02	0.142D-01	0.646D 00
0.750D 02	0.135D-01	0.662D 00
0.800D 02	0.130D-01	0.676D 00
0.850D 02	0.124D-01	0.689D 00
0.900D 02	0.120D-01	0.701D 00
0.950D 02	0.115D-01	0.713D 00
0.100D 03	0.111D-01	0.723D 00



MILLSTONE 1 FLAMMABILITY LIMITS

APPENDIX C

CALCULATION OF EXTENT OF RADIOLYSIS NECESSARY TO REACH FLAMMABLE GAS CONCENTRATIONS

In order to perform a large number of scenario calculations (varying f_{Zr-H_2O} and ϵ_{H_2O}) which lead to flammable containment gas mixtures, a simple computer program was written (shown in Figure C-1).

The extent of the metal water reaction (in %) is input as $I = f_{Zr-H_2O} + 1$. The extent of radiolytic decomposition (in lbs.) is then varied in lb. increments starting at 1.0 lb. until the $[H_2]_c$ (in %) crosses into the flammable region. When this occurs, the calculation is stopped. The last printed value of ϵH_2O corresponds to the extent of radiolysis required to yield a flammable containment gas concentration. Roughly 30 such calculations were subsequently carried out for varying f_{Zr-H_2O} values.

Figure C-2 is a typical output listing for the case of $f_{Zr-H_2O} = 14\%$. As noted on the final page of output, the necessary extent of radiolysis needed to yield flammable mixtures in 1980 lbs. Figure III of Section 3.2 summarizes the results of these calculations.

```
FORTRAN IV G LEVEL  21                MAIN              DATE = 82146        10/21/35            PAGE 0001

       C
       C        CALCULATION OF LBS. OF H2O THAT MUST DECOMPOSE.
       C                  JOHN BICKEL
       C
                REAL*8 CH,CO,X,F
                I = 15
                M=1
             30 CONTINUE
             20 F=DFLOAT(I-1) * .1D-1
                CH=(2.D0*F*3.52916D5 + M*25.178D0 + 2.7085D2)/
              A    (2.D0*F*3.52916D5 + M*37.767D0 + 2.7085D5)
                CH = CH * 1.0D2
                CO = (M*12.589D0 + 1.0834D4) /
              B       (2.D0*F*3.52916D5 + M*37.767D0 + 2.7085D5)
                Y = CO * 1.0D2
                CO = CO * .1D-1
                X = -0.7119376D2 + .2020868D2*Y -0.1054300D1*Y**2
              C     +0.1990303D-1*Y**3
                IF (CH.LE.X) GO TO 60
                M=M+1
                WRITE (6,100) M,F,CH,Y,X
            100 FORMAT(5X,I5,4(5X,D10.3))
                GO TO 30
             60 CONTINUE
                STOP
                END
```

FIG. C-1

$\mathcal{E}_{H_2O}$	f_{Zr-H_2O}	$[H_2]_c$	$[O_2]_c$	$[H_2]_{lim}$
2	0.140D 00	0.268D 02	0.293E 01	-0.205D 02
3	0.140D 00	0.268D 02	0.294E 01	-0.204D 02
4	0.140D 00	0.268D 02	0.294E 01	-0.204D 02
5	0.140D 00	0.268D 02	0.294E 01	-0.203D 02
6	0.140D 00	0.268D 02	0.295E 01	-0.203D 02
7	0.140D 00	0.268D 02	0.295E 01	-0.203D 02
8	0.140D 00	0.268D 02	0.295E 01	-0.202D 02
9	0.140D 00	0.268D 02	0.296E 01	-0.202D 02
10	0.140D 00	0.268D 02	0.296E 01	-0.201D 02
11	0.140D 00	0.268D 02	0.296E 01	-0.201D 02
12	0.140D 00	0.268D 02	0.296E 01	-0.200D 02
13	0.140D 00	0.269D 02	0.297E 01	-0.200D 02
14	0.140D 00	0.269D 02	0.297E 01	-0.199D 02
15	0.140D 00	0.269D 02	0.297E 01	-0.199D 02
16	0.140D 00	0.269D 02	0.298E 01	-0.198D 02
17	0.140D 00	0.269D 02	0.298E 01	-0.198D 02
18	0.140D 00	0.269D 02	0.298E 01	-0.198D 02
19	0.140D 00	0.269D 02	0.299E 01	-0.197D 02
20	0.140D 00	0.269D 02	0.299E 01	-0.197D 02
21	0.140D 00	0.269D 02	0.299E 01	-0.196D 02
22	0.140D 00	0.269D 02	0.300E 01	-0.196D 02
23	0.140D 00	0.269D 02	0.300E 01	-0.195D 02
24	0.140D 00	0.269D 02	0.300E 01	-0.195D 02
25	0.140D 00	0.269D 02	0.301E 01	-0.194D 02
26	0.140D 00	0.269D 02	0.301E 01	-0.194D 02
27	0.140D 00	0.269D 02	0.301E 01	-0.194D 02
28	0.140D 00	0.269D 02	0.301E 01	-0.193D 02
29	0.140D 00	0.269D 02	0.302E 01	-0.193D 02
30	0.140D 00	0.269D 02	0.302E 01	-0.192D 02
31	0.140D 00	0.269D 02	0.302E 01	-0.192D 02
32	0.140D 00	0.269D 02	0.303E 01	-0.191D 02
33	0.140D 00	0.269D 02	0.303E 01	-0.191D 02
34	0.140D 00	0.269D 02	0.303E 01	-0.190D 02
35	0.140D 00	0.269D 02	0.304E 01	-0.190D 02
36	0.140D 00	0.269D 02	0.304E 01	-0.190D 02
37	0.140D 00	0.270D 02	0.304E 01	-0.189D 02
38	0.140D 00	0.270D 02	0.305E 01	-0.189D 02
39	0.140D 00	0.270D 02	0.305E 01	-0.188D 02
40	0.140D 00	0.270D 02	0.305E 01	-0.188D 02
41	0.140D 00	0.270D 02	0.305E 01	-0.187D 02
42	0.140D 00	0.270D 02	0.306E 01	-0.187D 02
43	0.140D 00	0.270D 02	0.306E 01	-0.186D 02
44	0.140D 00	0.270D 02	0.306E 01	-0.186D 02
45	0.140D 00	0.270D 02	0.307E 01	-0.186D 02
46	0.140D 00	0.270D 02	0.307E 01	-0.185D 02
47	0.140D 00	0.270D 02	0.307E 01	-0.185D 02
48	0.140D 00	0.270D 02	0.308E 01	-0.184D 02
49	0.140D 00	0.270D 02	0.308E 01	-0.184D 02
50	0.140D 00	0.270D 02	0.308E 01	-0.183D 02
51	0.140D 00	0.270D 02	0.309E 01	-0.183D 02
52	0.140D 00	0.270D 02	0.309E 01	-0.183D 02
53	0.140D 00	0.270D 02	0.309E 01	-0.182D 02
54	0.140D 00	0.270D 02	0.309E 01	-0.182D 02
55	0.140D 00	0.270D 02	0.310E 01	-0.181D 02
56	0.140D 00	0.270D 02	0.310E 01	-0.181D 02
57	0.140D 00	0.270D 02	0.310E 01	-0.180D 02
58	0.140D 00	0.270D 02	0.311E 01	-0.180D 02
59	0.140D 00	0.270D 02	0.311E 01	-0.179D 02
60	0.140D 00	0.270D 02	0.311E 01	-0.179D 02

FIG. C-2

```
 61     0.140D 00     0.270D 02     0.312E 01     -0.179D 02
 62     0.140D 00     0.271D 02     0.312E 01     -0.178D 02
 63     0.140D 00     0.271D 02     0.312E 01     -0.178D 02
 64     0.140D 00     0.271D 02     0.313E 01     -0.177D 02
 65     0.140D 00     0.271D 02     0.313E 01     -0.177D 02
 66     0.140D 00     0.271D 02     0.313E 01     -0.176D 02
 67     0.140D 00     0.271D 02     0.313E 01     -0.176D 02
 68     0.140D 00     0.271D 02     0.314E 01     -0.176D 02
 69     0.140D 00     0.271D 02     0.314E 01     -0.175D 02
 70     0.140D 00     0.271D 02     0.314E 01     -0.175D 02
 71     0.140D 00     0.271D 02     0.315E 01     -0.174D 02
 72     0.140D 00     0.271D 02     0.315E 01     -0.174D 02
 73     0.140D 00     0.271D 02     0.315E 01     -0.173D 02
 74     0.140D 00     0.271D 02     0.316E 01     -0.173D 02
 75     0.140D 00     0.271D 02     0.316E 01     -0.173D 02
 76     0.140D 00     0.271D 02     0.316E 01     -0.172D 02
 77     0.140D 00     0.271D 02     0.316E 01     -0.172D 02
 78     0.140D 00     0.271D 02     0.317E 01     -0.171D 02
 79     0.140D 00     0.271D 02     0.317E 01     -0.171D 02
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 81     0.140D 00     0.271D 02     0.318E 01     -0.170D 02
 82     0.140D 00     0.271D 02     0.318E 01     -0.169D 02
 83     0.140D 00     0.271D 02     0.318E 01     -0.169D 02
 84     0.140D 00     0.271D 02     0.319E 01     -0.169D 02
 85     0.140D 00     0.271D 02     0.319E 01     -0.168D 02
 86     0.140D 00     0.271D 02     0.319E 01     -0.168D 02
 87     0.140D 00     0.272D 02     0.320E 01     -0.167D 02
 88     0.140D 00     0.272D 02     0.320E 01     -0.167D 02
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 90     0.140D 00     0.272D 02     0.320E 01     -0.166D 02
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 93     0.140D 00     0.272D 02     0.321E 01     -0.165D 02
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 95     0.140D 00     0.272D 02     0.322E 01     -0.164D 02
 96     0.140D 00     0.272D 02     0.322E 01     -0.163D 02
 97     0.140D 00     0.272D 02     0.323E 01     -0.163D 02
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 99     0.140D 00     0.272D 02     0.323E 01     -0.162D 02
100     0.140D 00     0.272D 02     0.324E 01     -0.162D 02
101     0.140D 00     0.272D 02     0.324E 01     -0.161D 02
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115     0.140D 00     0.273D 02     0.328E 01     -0.155D 02
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117     0.140D 00     0.273D 02     0.329E 01     -0.155D 02
118     0.140D 00     0.273D 02     0.329E 01     -0.154D 02
119     0.140D 00     0.273D 02     0.329E 01     -0.154D 02
120     0.140D 00     0.273D 02     0.330E 01     -0.153D 02
```

```
 121      0.140D 00      0.273D 02      0.330E 01      -0.153D 02
 122      0.140D 00      0.273D 02      0.330E 01      -0.152D 02
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 124      0.140D 00      0.273D 02      0.331E 01      -0.152D 02
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 126      0.140D 00      0.273D 02      0.331E 01      -0.151D 02
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 132      0.140D 00      0.273D 02      0.333E 01      -0.148D 02
 133      0.140D 00      0.273D 02      0.334E 01      -0.148D 02
 134      0.140D 00      0.273D 02      0.334E 01      -0.147D 02
 135      0.140D 00      0.273D 02      0.334E 01      -0.147D 02
 136      0.140D 00      0.273D 02      0.334E 01      -0.147D 02
 137      0.140D 00      0.274D 02      0.335E 01      -0.146D 02
 138      0.140D 00      0.274D 02      0.335E 01      -0.146D 02
 139      0.140D 00      0.274D 02      0.335E 01      -0.145D 02
 140      0.140D 00      0.274D 02      0.336E 01      -0.145D 02
 141      0.140D 00      0.274D 02      0.336E 01      -0.144D 02
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726    0.140D 00    0.296D 02    0.503E 01    0.628D 01
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728    0.140D 00    0.296D 02    0.503E 01    0.634D 01
729    0.140D 00    0.296D 02    0.504E 01    0.637D 01
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731    0.140D 00    0.296D 02    0.504E 01    0.643D 01
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1018     0.140D 00     0.306D 02     0.579E 01     0.144D 02
1019     0.140D 00     0.306D 02     0.579E 01     0.144D 02
1020     0.140D 00     0.306D 02     0.580E 01     0.144D 02
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1101    0.140D 00    0.308D 02    0.600E 01    0.164D 02
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1316      0.140D 00      0.315D 02      0.653E 01      0.214D 02
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1318      0.140D 00      0.315D 02      0.654E 01      0.214D 02
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1320      0.140D 00      0.315D 02      0.654E 01      0.215D 02
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1597     0.140D 00     0.324D 02     0.719E 01     0.270D 02
1598     0.140D 00     0.324D 02     0.720E 01     0.270D 02
1599     0.140D 00     0.324D 02     0.720E 01     0.271D 02
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1602     0.140D 00     0.324D 02     0.720E 01     0.271D 02
1603     0.140D 00     0.324D 02     0.721E 01     0.271D 02
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1607     0.140D 00     0.324D 02     0.722E 01     0.272D 02
1608     0.140D 00     0.324D 02     0.722E 01     0.272D 02
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1616     0.140D 00     0.325D 02     0.724E 01     0.274D 02
1617     0.140D 00     0.325D 02     0.724E 01     0.274D 02
1618     0.140D 00     0.325D 02     0.724E 01     0.274D 02
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1620     0.140D 00     0.325D 02     0.725E 01     0.275D 02
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1624      0.140D 00      0.325D 02      0.725E 01      0.275D 02
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1646      0.140D 00      0.325D 02      0.731E 01      0.279D 02
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1672      0.140D 00      0.326D 02      0.736E 01      0.284D 02
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1677      0.140D 00      0.326D 02      0.738E 01      0.285D 02
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1702    0.140D 00    0.327D 02    0.743E 01    0.289D 02
1703    0.140D 00    0.327D 02    0.743E 01    0.290D 02
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1879      0.140D 00      0.332D 02      0.782E 01      0.319D 02
1880      0.140D 00      0.332D 02      0.783E 01      0.319D 02
1881      0.140D 00      0.332D 02      0.783E 01      0.320D 02
1882      0.140D 00      0.332D 02      0.783E 01      0.320D 02
1883      0.140D 00      0.332D 02      0.783E 01      0.320D 02
1884      0.140D 00      0.332D 02      0.784E 01      0.320D 02
1885      0.140D 00      0.332D 02      0.784E 01      0.320D 02
1886      0.140D 00      0.332D 02      0.784E 01      0.320D 02
1887      0.140D 00      0.332D 02      0.784E 01      0.320D 02
1888      0.140D 00      0.332D 02      0.784E 01      0.321D 02
1889      0.140D 00      0.333D 02      0.785E 01      0.321D 02
1890      0.140D 00      0.333D 02      0.785E 01      0.321D 02
1891      0.140D 00      0.333D 02      0.785E 01      0.321D 02
1892      0.140D 00      0.333D 02      0.785E 01      0.321D 02
1893      0.140D 00      0.333D 02      0.786E 01      0.321D 02
1894      0.140D 00      0.333D 02      0.786E 01      0.322D 02
1895      0.140D 00      0.333D 02      0.786E 01      0.322D 02
1896      0.140D 00      0.333D 02      0.786E 01      0.322D 02
1897      0.140D 00      0.333D 02      0.786E 01      0.322D 02
1898      0.140D 00      0.333D 02      0.787E 01      0.322D 02
1899      0.140D 00      0.333D 02      0.787E 01      0.322D 02
1900      0.140D 00      0.333D 02      0.787E 01      0.323D 02
1901      0.140D 00      0.333D 02      0.787E 01      0.323D 02
1902      0.140D 00      0.333D 02      0.788E 01      0.323D 02
1903      0.140D 00      0.333D 02      0.788E 01      0.323D 02
1904      0.140D 00      0.333D 02      0.788E 01      0.323D 02
1905      0.140D 00      0.333D 02      0.788E 01      0.323D 02
1906      0.140D 00      0.333D 02      0.788E 01      0.324D 02
1907      0.140D 00      0.333D 02      0.789E 01      0.324D 02
1908      0.140D 00      0.333D 02      0.789E 01      0.324D 02
1909      0.140D 00      0.333D 02      0.789E 01      0.324D 02
1910      0.140D 00      0.333D 02      0.789E 01      0.324D 02
1911      0.140D 00      0.333D 02      0.789E 01      0.324D 02
1912      0.140D 00      0.333D 02      0.790E 01      0.324D 02
1913      0.140D 00      0.333D 02      0.790E 01      0.325D 02
1914      0.140D 00      0.333D 02      0.790E 01      0.325D 02
1915      0.140D 00      0.333D 02      0.790E 01      0.325D 02
1916      0.140D 00      0.333D 02      0.791E 01      0.325D 02
1917      0.140D 00      0.333D 02      0.791E 01      0.325D 02
1918      0.140D 00      0.333D 02      0.791E 01      0.325D 02
1919      0.140D 00      0.333D 02      0.791E 01      0.326D 02
1920      0.140D 00      0.333D 02      0.791E 01      0.326D 02
```

```
1921      0.140D 00      0.333D 02      0.792E 01      0.326D 02
1922      0.140D 00      0.333D 02      0.792E 01      0.326D 02
1923      0.140D 00      0.333D 02      0.792E 01      0.326D 02
1924      0.140D 00      0.334D 02      0.792E 01      0.326D 02
1925      0.140D 00      0.334D 02      0.793E 01      0.327D 02
1926      0.140D 00      0.334D 02      0.793E 01      0.327D 02
1927      0.140D 00      0.334D 02      0.793E 01      0.327D 02
1928      0.140D 00      0.334D 02      0.793E 01      0.327D 02
1929      0.140D 00      0.334D 02      0.793E 01      0.327D 02
1930      0.140D 00      0.334D 02      0.794E 01      0.327D 02
1931      0.140D 00      0.334D 02      0.794E 01      0.327D 02
1932      0.140D 00      0.334D 02      0.794E 01      0.328D 02
1933      0.140D 00      0.334D 02      0.794E 01      0.328D 02
1934      0.140D 00      0.334D 02      0.794E 01      0.328D 02
1935      0.140D 00      0.334D 02      0.795E 01      0.328D 02
1936      0.140D 00      0.334D 02      0.795E 01      0.328D 02
1937      0.140D 00      0.334D 02      0.795E 01      0.328D 02
1938      0.140D 00      0.334D 02      0.795E 01      0.328D 02
1939      0.140D 00      0.334D 02      0.796E 01      0.329D 02
1940      0.140D 00      0.334D 02      0.796E 01      0.329D 02
1941      0.140D 00      0.334D 02      0.796E 01      0.329D 02
1942      0.140D 00      0.334D 02      0.796E 01      0.329D 02
1943      0.140D 00      0.334D 02      0.796E 01      0.329D 02
1944      0.140D 00      0.334D 02      0.797E 01      0.329D 02
1945      0.140D 00      0.334D 02      0.797E 01      0.330D 02
1946      0.140D 00      0.334D 02      0.797E 01      0.330D 02
1947      0.140D 00      0.334D 02      0.797E 01      0.330D 02
1948      0.140D 00      0.334D 02      0.797E 01      0.330D 02
1949      0.140D 00      0.334D 02      0.798E 01      0.330D 02
1950      0.140D 00      0.334D 02      0.798E 01      0.330D 02
1951      0.140D 00      0.334D 02      0.798E 01      0.331D 02
1952      0.140D 00      0.334D 02      0.798E 01      0.331D 02
1953      0.140D 00      0.334D 02      0.799E 01      0.331D 02
1954      0.140D 00      0.334D 02      0.799E 01      0.331D 02
1955      0.140D 00      0.334D 02      0.799E 01      0.331D 02
1956      0.140D 00      0.334D 02      0.799E 01      0.331D 02
1957      0.140D 00      0.334D 02      0.799E 01      0.332D 02
1958      0.140D 00      0.334D 02      0.800E 01      0.332D 02
1959      0.140D 00      0.334D 02      0.800E 01      0.332D 02
1960      0.140D 00      0.335D 02      0.800E 01      0.332D 02
1961      0.140D 00      0.335D 02      0.800E 01      0.332D 02
1962      0.140D 00      0.335D 02      0.801E 01      0.332D 02
1963      0.140D 00      0.335D 02      0.801E 01      0.332D 02
1964      0.140D 00      0.335D 02      0.801E 01      0.333D 02
1965      0.140D 00      0.335D 02      0.801E 01      0.333D 02
1966      0.140D 00      0.335D 02      0.801E 01      0.333D 02
1967      0.140D 00      0.335D 02      0.802E 01      0.333D 02
1968      0.140D 00      0.335D 02      0.802E 01      0.333D 02
1969      0.140D 00      0.335D 02      0.802E 01      0.333D 02
1970      0.140D 00      0.335D 02      0.802E 01      0.334D 02
1971      0.140D 00      0.335D 02      0.802E 01      0.334D 02
1972      0.140D 00      0.335D 02      0.803E 01      0.334D 02
1973      0.140D 00      0.335D 02      0.803E 01      0.334D 02
1974      0.140D 00      0.335D 02      0.803E 01      0.334D 02
1975      0.140D 00      0.335D 02      0.803E 01      0.334D 02
1976      0.140D 00      0.335D 02      0.804E 01      0.334D 02
1977      0.140D 00      0.335D 02      0.804E 01      0.335D 02
1978      0.140D 00      0.335D 02      0.804E 01      0.335D 02
1979      0.140D 00      0.335D 02      0.804E 01      0.335D 02
1980      0.140D 00      0.335D 02      0.804E 01      0.335D 02
```

APPENDIX D

CALCULATION OF THE IMPACTS OF VAPOR PHASE H_2-O_2 RECOMBINATION

In Section 3.3.1 of Volume I, calculations are made assuming that during boiling phase (post-accident), there is a net production of H_2 and O_2 gases without any vapor phase recombination. In order to assess the level of conservatism employed in this approach, it is necessary to understand just how significant the vapor phase recombination (being omitted as a conservatism) actually is. Benjamin and Isben* experimentally measured the recombination rate of H_2 and O_2 (in water vapor) exposed to γ-radiation.

As a result of their measurements, the rate of recombination may be expressed as follows:

$$-\frac{d}{dt} p_{O_2} = \frac{k_0}{2} D_\gamma^{1/2} p_{H_2} p_{O_2}^{1/2} \qquad \text{(D-1)}$$

where: P_{H_2}, P_{O_2} are respectively the partial pressures of hydrogen and oxygen gas in atmospheres at 25°C.

k_0 is a rate constant equal to 4.394×10^{-12}.

D_γ is the dose rate per gm H_2O in units of eV/sec $\cdot$gmH_2O

$-\dfrac{dp_{H_2}}{dt}$ is the rate of removal for H_2 in atmospheres/sec.

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*Benjamin, B. M., and Isben, H. S., "Recombination of Hydrogen and Oxygen in the Presence of Water Vapor Under the Influence of Radiation," Final Report, AEC Contract AT (11-1)-1032, issued July 1965.

- To establish a perspective on the impacts of vapor phase recombination it is useful to compare the amount of recombination that occurs while steam is ~~in~~ near the core vs. the amount of H_2 and O_2 generated.

- Clearly this process is heavily dependent on the residence time of steam, H_2, and O_2 in the reactor vessel — where the γ dose is highest. By noting that non-condensibles (H_2 and O_2) are entrained in steam — the total residence time will be:

$$\tau_R = \frac{\text{steam volume}}{\text{volumetric steam flow rate}} = \frac{V_{st}}{v_s \cdot \dot{W}_s} \qquad \text{(D-2)}$$

-where: v_s is the specific volume of steam
V_{st} is the volume of the steam region
$\dot{W}_s$ is the steam mass flow rate.

Note that large $\dot{W}_s$ tends to reduce τ_R (as one would expect).

- A net equation for O_2 buildup can be written based on the Isben-Benjamin data as follows:

$$\frac{d}{dt} p_{O_2} = S_{O_2} - \frac{k_o}{2} D_{st}^{1/2} \, p_{H_2} \, p_{O_2}^{1/2} \qquad \text{(D-3)}$$

(a similar equation could be written describing p_{H_2}).

- By noting that $2H_2O \rightarrow 2H_2 + O_2$ then $p_{H_2} = 2p_{O_2}$ based on stoichiometry. Also:

$$S_{O_2} = \frac{\dot{n}_{O_2} RT}{V_{st}} \qquad \text{(D-4)}$$

- where: $\dot{n}_{O_2}$ is rate of evolution of O_2 via boiling radiolysis.

→

$$\dot{n}_{O_2} = \frac{V_{liq} \, D_{liq} \left(\frac{eV}{liter \cdot sec}\right) [illegible] \, G_{O_2} \left(\frac{molecules}{100\,eV}\right)}{100 \, A_o}$$

$A_o = 6.023 \times 10^{23} \frac{molecules}{mole}$ or Avogadro's number.

- The differential equation describing O_2 buildup is non-linear but may be solved via substitution—as follows:

$$\frac{d}{dt} p_{O_2} = S_{O_2} - \frac{k_0}{2} D_{st}^{1/2} 2 p_{O_2}^{3/2} \qquad (D-5)$$

- becomes upon rearranging:

$$d p_{O_2} - S_{O_2}\, dt = -k_0 D_{st}^{1/2} p_{O_2}^{3/2}\, dt$$

$$d[p_{O_2} e^{-S_{O_2} t}] = -k_0 D_{st}^{1/2} p_{O_2}^{3/2}\, dt \qquad (D-6)$$

- defining $z(t) = p_{O_2} e^{-S_{O_2} t}$, Equation D-6 becomes:

$$\frac{d[z(t)]}{z(t)^{3/2}} = -k_0 D_{st}^{1/2} e^{3S_{O_2} t/2}\, dt \qquad (D-7)$$

Integrating this equation between 0 and τ_R (the total time available for any recombination to take place) yields the following expression:

$$-2z(\tau_R)^{-1/2} + 2z(0)^{-1/2} = -k_0 D_{st}^{1/2} \int_0^{\tau_R} e^{3S_{O_2} t/2}\, dt$$

$$= -k_0 D_{st}^{1/2} \left(\frac{2}{3S_{O_2}}\right) e^{3S_{O_2}\tau_R/2} \qquad (D-8)$$

Solving for $z(\tau_R)$ yields:

$$z(\tau_R) = \frac{1}{\left[z(0)^{-1/2} + \frac{k_0 D_{st}^{1/2}}{3S_{O_2}} e^{3S_{O_2}\tau_R/2}\right]^2} \qquad (D-9)$$

o Noting that: $z(0) = p(0) = 0$ and $z(\tau_R) = \rho_{O_2}(\tau_R)\, e^{-S_{O_2}\tau_R}$

Equation D-9 becomes:

$$\Delta\rho_{O_2}(\tau_R) = \frac{e^{S_{O_2}\tau_R}}{\frac{k_o^2 D_{st}}{3^2 S_{O_2}^2}\, e^{3S_{O_2}\tau_R}}$$

$$= \frac{9 S_{O_2}^2 e^{-2S_{O_2}\tau_R}}{k_o^2 D_{st}} = \frac{9 S_{O_2}^2 e^{-2S_{O_2} V_{st}/N_s \dot{W}_s}}{k_o^2 D_{st}} \quad \text{(D-10)}$$

o This expression may be compared to the predicted ρ_{O_2} if no vapor phase recombination were assumed during the same time frame:

$$\frac{d}{dt}\rho_{O_2} = S_{O_2} \quad \text{OR: } \Delta\rho_{O_2}(\tau_R) = S_{O_2}\tau_R \quad \text{(D-11)}$$

$$= \frac{S_{O_2} V_{st}}{N_s \dot{W}_s}$$

o To perform some simple calculations assume:

$V_{tot} \cong 4.052 \times 10^5$ liters , $T \cong 100°C$ (barely subcooled)

$\frac{V_{liq}}{V_{tot}} \cong .5$, $D_{liq} = 1 \times 10^{18} \frac{eV}{liter \cdot sec}$, $N_s = 1.673 \frac{liter}{gram}$

$$^{*}\ \frac{D_{st}}{N_s} = 1 \times 10^{16} \frac{eV}{liter \cdot sec} \cdot \frac{1}{1.673 \frac{liter}{gr}} = 5.98 \times 10^{15} \frac{eV}{gr \cdot sec}$$

---

* The calculation of steam dose requires a more detailed evaluation - for the purposes of this "quick" evaluation it is assumed steam dose is ~ 10^{-2} of liquid doses. Further detailed analysis should be performed if this item were critical. In this study it is not.

° If it were assumed that: $\dot{W}_S = 1.0 \text{ lbs/sec} = 4.536\times10^2 \frac{\text{gr}}{\text{sec}}$

$$S_{O_2} = \frac{V_{liq} \cdot D_{liq} \cdot G_{O_2} \cdot RT}{100\, A_o\, V_{st}} \qquad (V_{liq} \cong V_{st})$$

$$= \frac{\left(1\times10^{18} \frac{\text{eV}}{\text{liter}\cdot\text{sec}}\right)\left(0.22 \frac{\text{molecules}}{100\text{ eV}}\right)(.08205)(298.15\,°\text{K})}{(100)\left(6.023\times10^{23}\frac{\text{molecules}}{\text{mole}}\right)}$$

$$= 8.94\times10^{-8}\ \frac{\text{atmospheres } O_2}{\text{sec.}} \qquad (D\text{-}12)$$

- Assuming *no* vapor phase recombination takes place, during the time period the steam, H_2, + O_2 gas are in the steam volume, the net partial pressure added during τ_R would be:

$$\Delta p(\tau_R) = S_{O_2}\tau_R = S_{O_2}\cdot\frac{V_{st}}{v_s\,\dot{W}_s}$$

$$= \frac{\left(8.94\times10^{-8}\frac{\text{atmos.}}{\text{sec}}\right)\left(2.02588\times10^{5} \text{ liters}\right)}{\left(1.673 \text{ liters/gram}\right)\left(4.536\times10^{2}\text{ gr/sec}\right)}$$

$$= 2.386\times10^{-5} \text{ atmospheres } O_2 \qquad (D\text{-}13)$$

- For the same time period, if it were assumed that vapor phase recombination were occurring:

$$\Delta p(\tau_R) = \frac{9 S_{O_2}^2 e^{-2 S_{O_2} V_{st}/v_s \cdot \dot{W}_s}}{k_o^2\, D_{st}}$$

$$= \frac{(9)(8.94\times10^{-8})^2 \exp\left(-2(2.386\times10^{-5})\right)}{(4.394\times10^{-12})^2\left(5.98\times10^{15}\frac{\text{eV}}{\text{gr-sec}}\right)}$$

$$= 6.23\times10^{-7} \text{ atmospheres } O_2 \qquad (D\text{-}14)$$

The effectiveness of recombination for these conditions is a result of having a very <u>small</u> steam mass flow rate out of the vessel, hence a very substantial portion of the gases have time to recombine. The more likely situation is for higher mass flow rates which transport steam, H_2, and O_2 out of the vessel before the H_2 and O_2 can recombine. Thus assume $\dot{W}_S = 10.$ lbs/sec. $= 4.536 \times 10^3$ gr/sec.

If no vapor phase recombination is assumed $\Delta \rho_{O_2}$ during the time $\tau_R = \frac{V_{st}}{v_S \cdot \dot{W}_S}$ would be:

$$\Delta \rho_{O_2}(\tau_r) = S_{O_2} \frac{V_{st}}{v_S \cdot \dot{W}_S}$$

$$= \frac{\left(8.94 \times 10^{-8} \frac{\text{atmos}}{\text{sec.}}\right)\left(2.02588 \times 10^5 \text{ liters}\right)}{\left(1.673 \text{ liters/gram}\right)\left(4.536 \times 10^3 \text{ gr/sec}\right.}$$

$$= 2.386 \times 10^{-6} \text{ atmospheres } O_2 \qquad (D\text{-}15)$$

Recalculating the impacts of this steam flow for the case where recombination is assumed yields:

$$\Delta \rho_{O_2}(\tau_R) = \frac{9 (S_{O_2})^2 e^{-2 S_{O_2} V_{st}/v_S \cdot \dot{W}_S}}{k_0^2 \; D_{st}}$$

$$= \frac{9(8.94 \times 10^{-8})^2 \exp\left[-2.(2.386 \times 10^{-6})\right]}{(4.394 \times 10^{-12})^2 (5.98 \times 10^{15} \text{ eV/gr} \cdot \text{sec})}$$

$$\cong 6.23 \times 10^{-7}$$

thus roughly the same amount of recombination occurs.

These simplified calculations indicate the following:

- If steam flow rates are slow enough, and if γ dose rates are appreciably high a considerable portion of the radiolytically evolved H_2 and O_2 can recombine when exposed to the radiation from the core.
- To take credit for this effect, however, it is necessary to develop scenario dependent: V_{st}, V_{liq}, D_{st}, D_{liq}, and temperature values.
- As steam flows are increased, the H_2 and O_2 have insufficient time to recombine while above the core. (Normal operation, and rapid steam blow down are good cases of this type of situation)
- Omission of this effect (e.g. vapor phase H_2 and O_2 recombination in a γ-radiation field) will provide varying degrees of conservatism during the boiling phase of a hypothetical accident or transient, because net H_2 and O_2 production will be slightly larger, dependent on steam flows.

APPENDIX E

CALCULATION OF RADIOLYTIC DECOMPOSITION WITH EXPOSURE, NEGLECTING VAPOR PHASE RECOMBINATION

In order to perform sensitivity studies on the extent of radiolysis and the impacts of changes in the dominant parameters, a short computer program was written to evaluate the following equation derived in Section 3.3.1 of Volume I:

$$M_{H_2O}(t) = A_o P_o f_{\beta,\gamma} (G_{H_2} m_{H_2} + G_{O_2} m_{O_2}) \sum_i \frac{k_i}{\lambda_i} (1 - e^{-\lambda_i t}) \tag{E-1}$$

(constants k_i, λ_i are specified in Section 3.3.1 based on NRC Reg. Guide 1.7)

In this program the following inputs are utilized:

Variable	Definition	Units
PO	Initial thermal power	MW_t
FBG	$f_{\beta,\gamma}$ fraction of β, γ energy absorbed in core coolant	(fraction)
GH2	G_{H_2}, Net radiolytic yield of H_2	molecules/100 eV

GO2 G_{O_2}, Net radiolytic yield of O_2 molecules/100 eV

The time values utilized in this calculation are input in an array: T and the calculation yields values of M_{H_2O} at times: T(i).

Three sample cases are hown and these are defined as follows:

CASE I (Conservative Lower Bound)

PO = 2.011×10^3 (Licensed Power)

FBG = .094

GH2 = 0.20

GO_2 = 0.10

- this case is conservative due to the fact that a high value for $f_{\beta, \gamma}$ is used corresponding to the coldest temperature.

Results of CASE I are shown in Figure E-1.

CASE II

PO = 2.011×10^3 (Licensed Power)

FBG = .094

GH2 = 0.20

GO2 = 0.10

Results of CASE II are shown in Figure E-2.

CASE III (Highly Conservative Upper Bound)

PO = 2.051 x 10^3 (102% Licensed Power)

FBG = .094

GH2 = 0.44

GO2 = 0.22

Results of CASE III are shown in Figure E-3.

```
FORTRAN IV G LEVEL  21                MAIN                  DATE = 82147          13/34/12                PAGE 0001
                C
                C       CALCULATION OF BOILING-PHASE RADIOLYTIC DECOMPOSTION OF WATER
                C                    JOHN BICKEL
                C       MAY 27, 1982
                C
 0001                   DIMENSION T(23),RADM(23)
 0002                   REAL*8 PO,FBG,GH2,GO2,F,RADM,T
 0003                   PO = 2.011D3
 0004                   FBG= 0.94D-1
 0005                   GH2= 0.20D0
 0006                   GO2= 0.10D0
 0007                   F  = 3.6526D-7 * (GH2 * 2.016D0 + GO2 * 3.1999D1) * FBG * PO
 0008                   DATA T/.1D0,.1D2,.1D3,.2D3,.5D3,.7D3,.1D4,
                      X        .2D4,.5D4,.7D4,.1D5,.2D5,.3D5,.4D5,
                      X        .5D5,.6D5,.7D5,.8D5,.9D5,.1D6,.2D6,.3D6,.5D6/
 0009                   DO 10 I = 1,23
 0010                   RADM(I) = (5.1912D0/9.8D-5) * (1D0-DEXP(-9.8D-5*T(I)))
                      X          + (0.8743D0/6.5D-6) * (1D0-DEXP(-6.5D-6*T(I)))
                      X          + (0.6557D0/5.7D-7) * (1D0-DEXP(-5.7D-7*T(I)))
                      X          + (0.4098D0/7.4D-8) * (1D0-DEXP(-7.4D-8*T(I)))
                      X          + (0.15D1/8.0D-10) * (1D0-DEXP(-8.0D-10*T(I)))
 0011                   RADM(I) = RADM(I) * F
 0012                10 WRITE(6,11) T(I),RADM(I)
 0013                11 FORMAT(5X,2(5X,D10.3))
 0014                   STOP
 0015                   END
```

CASE I

FIG. E-1

t (sec)	ε_{H_2O} (lbs.)
0.1000 00	0.215D-03
0.100D 02	0.215D-01
0.100D 03	0.214D 00
0.200D 03	0.427D 00
0.500D 03	0.106D 01
0.700D 03	0.147D 01
0.100D 04	0.209D 01
0.200D 04	0.405D 01
0.500D 04	0.936D 01
0.700D 04	0.125D 02
0.100D 05	0.167D 02
0.200D 05	0.281D 02
0.300D 05	0.375D 02
0.400D 05	0.460D 02
0.500D 05	0.542D 02
0.600D 05	0.621D 02
0.700D 05	0.698D 02
0.800D 05	0.775D 02
0.900D 05	0.850D 02
0.100D 06	0.925D 02
0.200D 06	0.163D 03
0.300D 06	0.229D 03
0.500D 06	0.353D 03

```
C
C     CALCULATION OF BOILING-PHASE RADIOLYTIC DECOMPOSTION OF WATER
C                JOHN BICKEL
C     MAY 27, 1982
C
      DIMENSION T(23),RADM(23)
      REAL*8 PO,FBG,GH2,GO2,F,RADM,T
      PO = 2.011D3
      FBG= 0.94D-1
      GH2= 0.44D0
      GO2= 0.22D0
      F  = 3.6526D-7 * (GH2 * 2.016D0 + GO2 * 3.1999D1) * FBG * PO
      DATA T/.1D0,.1D2,.1D3,.2D3,.5D3,.7D3,.1D4,
     X        .2D4,.5D4,.7D4,.1D5,.2D5,.3D5,.4D5,
     X        .5D5,.6D5,.7D5,.8D5,.9D5,.1D6,.2D6,.3D6,.5D6/
      DO 10 I = 1,23
      RADM(I) = (5.1912D0/9.8D-5) * (1D0-DEXP(-9.8D-5*T(I)))
     X          + (0.8743D0/6.5D-6) * (1D0-DEXP(-6.5D-6*T(I)))
     X          + (0.6557D0/5.7D-7) * (1D0-DEXP(-5.7D-7*T(I)))
     X          + (0.4098D0/7.4D-8) * (1D0-DEXP(-7.4D-8*T(I)))
     X          + (0.15D1/8.0D-10)  * (1D0-DEXP(-8.0D-10*T(I)))
      RADM(I) = RADM(I) * F
   10 WRITE(6,11) T(I),RADM(I)
   11 FORMAT(5X,2(5X,D10.3))
      STOP
      END
```

CASE II
FIG. E-2

t (sec)	ε_{H_2O} (lbs)
0.1000D 00	0.472D-03
0.1000D 02	0.472D-01
0.1000D 03	0.471D 00
0.2000D 03	0.939D 00
0.5000D 03	0.233D 01
0.7000D 03	0.324D 01
0.1000D 04	0.459D 01
0.2000D 04	0.892D 01
0.5000D 04	0.206D 02
0.7000D 04	0.275D 02
0.1000D 05	0.363D 02
0.2000D 05	0.619D 02
0.3000D 05	0.825D 02
0.4000D 05	0.101D 03
0.5000D 05	0.119D 03
0.6000D 05	0.137D 03
0.7000D 05	0.154D 03
0.8000D 05	0.170D 03
0.9000D 05	0.187D 03
0.1000D 06	0.204D 03
0.2000D 06	0.359D 03
0.3000D 06	0.504D 03
0.5000D 06	0.776D 03

```
FORTRAN IV G LEVEL  21                 MAIN              DATE = 82147          13/41/05               PAGE 0001
              C
              C      CALCULATION OF BOILING-PHASE RADIOLYTIC DECOMPOSTION OF WATER
              C               JOHN BICKEL
              C      MAY 27, 1982
              C
 0001                DIMENSION T(23),PADM(23)
 0002                REAL*8 PO,FBG,GH2,GO2,F,RADM,T
 0003                PO = 2.051D3
 0004                FBG= 0.94D-1
 0005                GH2= 0.44D0
 0006                GO2= 0.22D0
 0007                F  = 3.6526D-7 * (GH2 * 2.016D0 + GO2 * 3.1999D1) * FBG * PO
 0008                DATA T/.1D0,.1D2,.1D3,.2D3,.5D3,.7D3,.1D4,
                    X        .2D4,.5D4,.7D4,.1D5,.2D5,.3D5,.4D5,
                    X        .5D5,.6D5,.7D5,.8D5,.9D5,.1D6,.2D6,.3D6,.5D6/
 0009                DO 10 I = 1,23
 0010                RADM(I) = (5.1912D0/9.8D-5) * (1D0-DEXP(-9.8D-5*T(I)))
                    X         + (0.8743D0/6.5D-6) * (1D0-DEXP(-6.5D-6*T(I)))
                    X         + (0.6557D0/5.7D-7) * (1D0-DEXP(-5.7D-7*T(I)))
                    X         + (0.4098D0/7.4D-8) * (1D0-DEXP(-7.4D-8*T(I)))
                    X         + (0.15D1/8.0D-10)  * (1D0-DEXP(-8.0D-10*T(I)))
 0011                RADM(I) = RADM(I) * F
 0012             10 WRITE(6,11) T(I),RADM(I)
 0013             11 FORMAT(5X,2(5X,D10.3))
 0014                STOP
 0015                END
```

CASE III

FIG. E-3

t (sec) ε_{H_2O} (lbs)

```
0.100D 00      0.482D-03
0.100D 02      0.482D-01
0.100D 03      0.480D 00
0.200D 03      0.958D 00
0.500D 03      0.237D 01
0.700D 03      0.330D 01
0.100D 04      0.468D 01
0.200D 04      0.910D 01
0.500D 04      0.210D 02
0.700D 04      0.280D 02
0.100D 05      0.375D 02
0.200D 05      0.632D 02
0.300D 05      0.842D 02
0.400D 05      0.103D 03
0.500D 05      0.122D 03
0.600D 05      0.139D 03
0.700D 05      0.157D 03
0.800D 05      0.174D 03
0.900D 05      0.191D 03
0.100D 06      0.208D 03
0.200D 06      0.366D 03
0.300D 06      0.514D 03
0.500D 06      0.792D 03
```

APPENDIX F

CALCULATION OF POST BOILING PHASE H_2-O_2 CONCENTRATIONS

It is necessary to assess the impacts of short-term boiling phase radiolysis on containment gas concentrations for two reasons:

- An accurate definition of the ranges of possible containment gas concentrations allows one to readily determine the existing margin against flammability provided merely by containment inerting with excess N_2 gas.
- In order to perform an analysis of post-boiling phase radiolysis using detailed chemical reaction kinetics, it is necessary to properly define the initial conditions.

For the purposes of assessing flammability potential, the most conservative approach is to assume that all radiolytic gases generated remain in the containment gas volume (hence no dissolution into coolant water is assumed). Equations 3.17-3.18 (of Section 3.3.2 in Volume I) define the ranges of these possible gas concentrations. To facilitate determination of the limits defined by these equations, a simple program was written shown in Figure F-1 (along with numerical results). The numerical results are shown plotted in Figure F-2.

To examine the case where H_2 and O_2 redissolve into the subcooled water in the core and torus regions, another program was written which evaluates Equations 3.26a and 3.26b for various metal-water reactions and minimum/maximum boiling phase radiolysis. This program was run for 25°C 50°C, 75°C, and 100°C (shown as Figures F-3 through F-6).

```
FORTRAN IV G LEVEL  21                MAIN              DATE = 82165        12/19/10             PAGE 0001
               C
               C     CALCULATION OF POST-BOILING CONTAINMENT GAS CONCENTRATIONS
               C                JOHN BICKEL
               C     JUNE 1,1982
               C
 0001                DIMENSION FZR(12),CH2(12),CO2(12)
 0002                REAL*8 FZR,CH2,CO2
 0003                DATA FZR/0.D0, 1D-3, 2D-3, 5D-3, 6.125D-3, 7D-3,
                    X          1D-2, 5D-2, 1D-1, 2D-1, 3D-1, 5D-1/
 0004                DO 10 I = 1,12
 0005                CH2(I) = (FZR(I)*7.05832D5 + 3.04043D3) /(FZR(I) * 7.05832D5
                    X          + 2.75004D5)
 0006                CO2(I) = (1.22187D4)/(FZR(I)*7.05832D5 + 2.75004D5)
 0007             10 WRITE (6,11) FZR(I), CH2(I), CO2(I)
 0008             11 FORMAT(/10X,3(5X,D10.3))
 0009                DO 20 I = 1,12
 0010                CH2(I) = (FZR(I) * 7.05832D5 + 6.23342D2)/(FZR(I) * 7.05832D5
                    X          + 2.71378D5)
 0011                CO2(I) =  1.10102D4/(FZR(I) * 7.05832D5 + 2.71378D5)
 0012             20 WRITE (6,11) FZR(I), CH2(I), CO2(I)
 0013             21 FORMAT(/10X, 3(5X,D10.3))
 0014                STOP
 0015                END
```

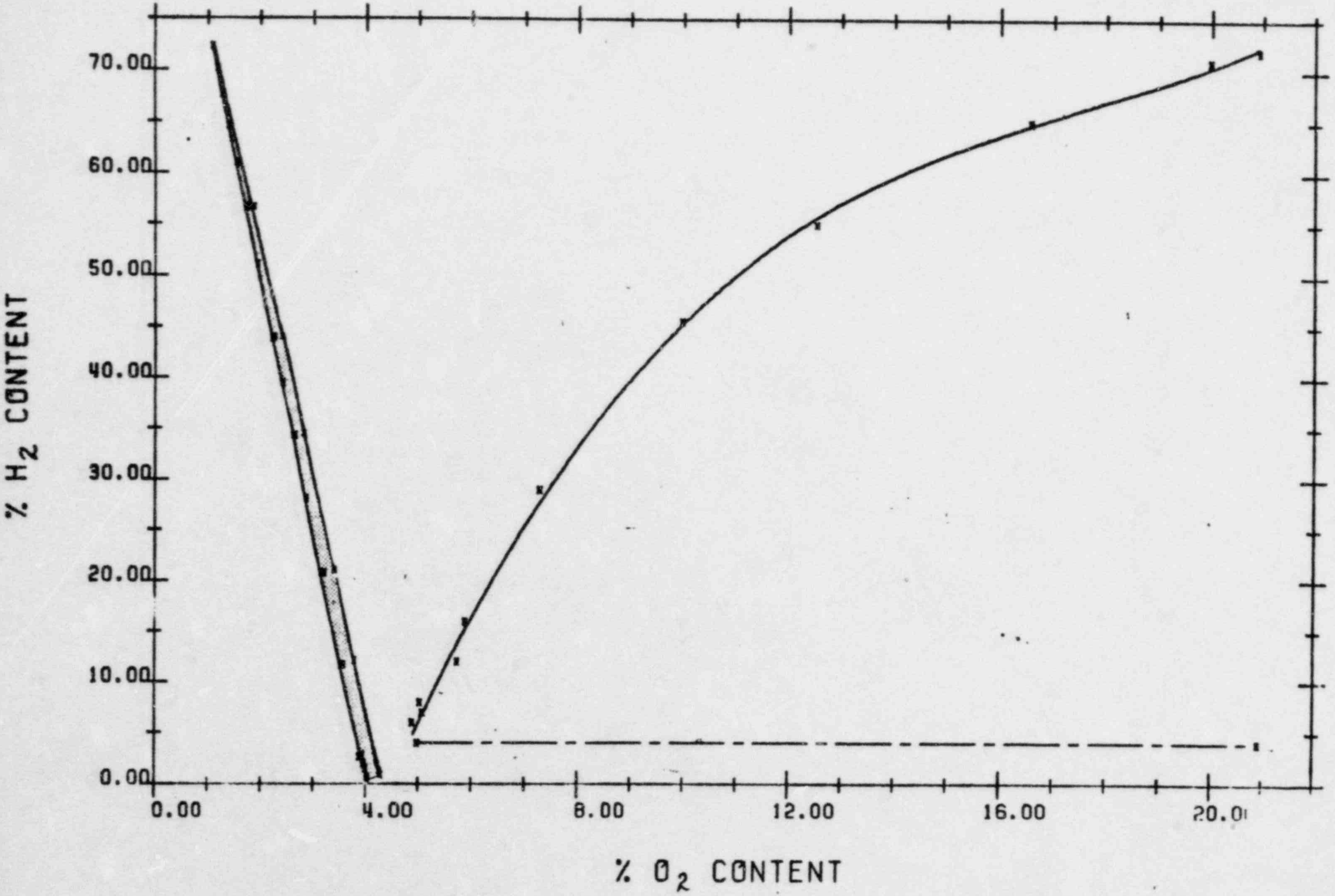
FIG. F-1

f_{Zr-H_2O}	$[H_2]_c$	$[O_2]_c$
0.0	0.111D-01	0.444D-01
0.100D-02	0.136D-01	0.443D-01
0.200D-02	0.161D-01	0.442D-01
0.500D-02	0.236D-01	0.439D-01
0.612D-02	0.264D-01	0.437D-01
0.700D-02	0.283D-01	0.436D-01
0.100D-01	0.358D-01	0.433D-01
0.500D-01	0.124D 00	0.394D-01
0.100D 00	0.213D 00	0.354D-01
0.200D 00	0.347D 00	0.294D-01
0.300D 00	0.441D 00	0.251D-01
0.500D 00	0.567D 00	0.195D-01

Assuming Maximum
Radiolysis : $\varepsilon_{H_2O} = 110$ lbs.

0.0	0.230D-02	0.406D-01
0.100D-02	0.489D-02	0.405D-01
0.200D-02	0.746D-02	0.404D-01
0.500D-02	0.151D-01	0.401D-01
0.612D-02	0.179D-01	0.399D-01
0.700D-02	0.201D-01	0.398D-01
0.100D-01	0.276D-01	0.395D-01
0.500D-01	0.117D 00	0.359D-01
0.100D 00	0.208D 00	0.322D-01
0.200D 00	0.344D 00	0.267D-01
0.300D 00	0.440D 00	0.228D-01
0.500D 00	0.566D 00	0.176D-01

Assuming Minimum
Radiolysis : $\varepsilon_{H_2O} = 14$ lbs.



RANGE OF POSSIBLE POST BOILING PHASE GAS CONCENTRATIONS

```
C
C     CALCULATION OF POST-BOILING PHASE DISSOLVED GAS
C     CONCENTRATIONS IN REACTOR COOLANT WATER AND CONTAINMENT
C                      JOHN BICKEL
C                      JUNE 8, 1982
C
C ********************************************************************
C
      DIMENSION FZR(12), CH2(12), CO2(12), PH2(12), PO2(12)
      REAL * 8 WH, WO, SH, SO ,VC, VL, R, T, GAMH, GAMO, FZR, MNE,
     X CH2, CO2, PH2, PO2
      DATA FZR /0.D0,1.D-3,2.D-3,5.D-3,6.125D-3, 7.D-3, 1.D-2, 5.D-2,
     X          1.D-1, 2.D-1, 3.D-1, 5.D-1/
C     CALCULATION OF MOLAR PARTITION COEFFICIENTS
C     WX = MOLECULAR WEIGHT IN GRAMS/MOLE
C     SX = SOLUBILITY IN MILLIGRAMS/LITER H2O
C     VC = CONTAINMENT VOLUME IN LITERS
C     VL = LIQUID VOLUME IN LITERS
C     R  = GAS LAW CONSTANT
C     T  = ABSOLUTE TEMPERATURE IN DEGREES KELVIN
C
C ********************************************************************
      WH = 2.016D0
      WO = 3.19981D1
      SH = 1.575D-3
      SO = 4.065D-2
      VC = 7.291D6
      VL = 2.605D6
      R  = 8.205D-2
      T  = 2.9815D2
      GAMH = (WH * VC ) / (SH * R * T * VL)
      GAMO = (WO * VC ) / (SO * R * T * VL)
      WRITE (6,10) GAMH, GAMO
   10 FORMAT(/,10X'H2 PART.COEFF. = ',D10.3,10X,'O2 PART.COEFF.=',D10.3)
C
C  CALCULATION OF H2 AND O2 CONCENTRATIONS FOR MINIMUM BOILING TIME
C
      EMN = 1.4D1
      WRITE (6,20) EMN
   20 FORMAT(/5X,'MINIMUM BOILING TIME CALC.--',D10.3,' LBS.DECOMPOSED')
      DO 45 I =1,12
      CH2(I) = (2.7085D2 + 2D0 * FZR(I) * 3.52916D5 + 2.5178D1 * EMN )
      PH2(I) = (CH2(I) * R * T) / VC
      CH2(I) = CH2(I) / (VL * (GAMH + 1D0))
      CO2(I) = (1.0834D4 + 1.2589D1 * EMN)
      PO2(I) = (CO2(I) * R * T)/VC
      CO2(I) = (CO2(I) / (VL * (GAMO + 1D0)))
   45 WRITE (6,50) FZR(I), CH2(I), PH2(I), CO2(I), PO2(I)
   50 FORMAT(/3X,'FRACT.ZR-H2O=',D10.3,3X,'(H2)=',D10.3,'MOLES/LITER',
     X 3X,'PH2=',D10.3,'ATMOS.',3X,'(O2)=',D10.3,'MOLES/LITER',3X,
     Y 'PO2=',D10.3,'ATMOS.')
C
C     CALCULATION OF H2 AND O2 CONCENTRATIONS FOR
```

CASE I

T=25°C

FIG. F-3

```
            C              MAXIMUM BOILING TIME                                 00000580
            C                                                                   00000590
 0028             EMX = 1.1D2                                                   00000600
 0029             WRITE(6,100)EMX                                               00000610
 0030         100 FORMAT(//5X,'MAXIMUM BOILING TIME CALC.--',D10.3,'LBS.DECOMPOSED')00000620
 0031             DO 25 I =1,12                                                 00000630
 0032             CH2(I) = (2.7085D2 + 2D0 * FZR(I) * 3.5291605 + 2.5178D1 * EMX )  00000640
 0033             PH2(I) = (CH2(I) * R * T) / VC                                00000650
 0034             CH2(I) = CH2(I) / (VL * (GAMH + 1D0))                         00000660
 0035             CO2(I) = (1.0834D4 + 1.2589D1 * EMX)                          00000670
 0036             PO2(I) = (CO2(I) * R * T)/VC                                  00000680
 0037             CO2(I) = (CO2(I) / (VL * (GAMO + 1D0)))                       00000690
 0038          25 WRITE (6,50) FZR(I), CH2(I), PH2(I), CO2(I), PO2(I)           00000700
 0039             STOP                                                          00000710
 0040             END                                                           00000720
```

```
     H2 PART.COEFF. =  0.146D 03          O2 PART.COEFF.= 0.901D 02
   MINIMUM BOILING TIME CALC.-- 0.140E 02 LBS.DECOMPOSED
 FRACT.ZR-H2O= 0.0          (H2)= 0.162D-05MOLES/LITER   PH2= 0.209D-02ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.100D-02    (H2)= 0.346D-05MOLES/LITER   PH2= 0.446D-02ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.200D-02    (H2)= 0.530D-05MOLES/LITER   PH2= 0.683D-02ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.500D-02    (H2)= 0.108D-04MOLES/LITER   PH2= 0.139D-01ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.612D-02    (H2)= 0.129D-04MOLES/LITER   PH2= 0.166D-01ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.700D-02    (H2)= 0.145D-04MOLES/LITER   PH2= 0.187D-01ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.100D-01    (H2)= 0.200D-04MOLES/LITER   PH2= 0.258D-01ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.500D-01    (H2)= 0.935D-04MOLES/LITER   PH2= 0.121D 00ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.100D 00    (H2)= 0.185D-03MOLES/LITER   PH2= 0.239D 00ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.200D 00    (H2)= 0.369D-03MOLES/LITER   PH2= 0.476D 00ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.300D 00    (H2)= 0.553D-03MOLES/LITER   PH2= 0.713D 00ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.
 FRACT.ZR-H2O= 0.500D 00    (H2)= 0.920D-03MOLES/LITER   PH2= 0.119D 01ATMOS.   (O2)= 0.464D-04MOLES/LITER   PO2= 0.369D-01ATMOS.

   MAXIMUM BOILING TIME CALC.-- 0.110E 03LBS.DECOMPOSED
 FRACT.ZR-H2O= 0.0          (H2)= 0.792D-05MOLES/LITER   PH2= 0.102D-01ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.100D-02    (H2)= 0.975D-05MOLES/LITER   PH2= 0.126D-01ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.200D-02    (H2)= 0.116D-04MOLES/LITER   PH2= 0.149D-01ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.500D-02    (H2)= 0.171D-04MOLES/LITER   PH2= 0.220D-01ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.612D-02    (H2)= 0.192D-04MOLES/LITER   PH2= 0.247D-01ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.700D-02    (H2)= 0.208D-04MOLES/LITER   PH2= 0.268D-01ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.100D-01    (H2)= 0.263D-04MOLES/LITER   PH2= 0.339D-01ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.500D-01    (H2)= 0.998D-04MOLES/LITER   PH2= 0.129D 00ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.100D 00    (H2)= 0.192D-03MOLES/LITER   PH2= 0.247D 00ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.200D 00    (H2)= 0.375D-03MOLES/LITER   PH2= 0.484D 00ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.300D 00    (H2)= 0.559D-03MOLES/LITER   PH2= 0.721D 00ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
 FRACT.ZR-H2O= 0.500D 00    (H2)= 0.927D-03MOLES/LITER   PH2= 0.119D 01ATMOS.   (O2)= 0.515D-04MOLES/LITER   PO2= 0.410D-01ATMOS.
```

CASE II

T=50°C

FIG. F-4

```
          C
          C     CALCULATION OF POST-BOILING PHASE DISSOLVED GAS
          C     CONCENTRATIONS IN REACTOR COOLANT WATER AND CONTAINMENT
          C                     JOHN BICKEL
          C                     JUNE 8, 1982
          C
          C ******************************************************************
          C
0001            DIMENSION FZR(12), CH2(12), CO2(12), PH2(12), PO2(12)
0002            REAL * 8 WH, WO, SH, SO ,VC, VL, R, T, GAMH, GAMO, FZR, MNE,
               X CH2, CO2, PH2, PO2
0003            DATA FZR /0.D0,1.D-3,2.D-3,5.D-3,6.125D-3, 7.D-3, 1.D-2, 5.D-2,
               X          1.D-1, 2.D-1, 3.D-1, 5.D-1/
          C     CALCULATION OF MOLAR PARTITION COEFFICIENTS
          C     WX = MOLECULAR WEIGHT IN GRAMS/MOLE
          C     SX = SOLUBILITY IN MILLIGRAMS/LITER H2O
          C     VC = CONTAINMENT VOLUME IN LITERS
          C     VL = LIQUID VOLUME IN LITERS
          C     R  = GAS LAW CONSTANT
          C     T  = ABSOLUTE TEMPERATURE IN DEGREES KELVIN
          C
          C ******************************************************************
0004            WH = 2.016D0
0005            WO = 3.19981D1
0006            SH = 1.48D-3
0007            SO = 2.99D-2
0008            VC = 7.291D6
0009            VL = 2.605D6
0010            R  = 8.205D-2
0011            T  = 3.2315D2
0012            GAMH = (WH * VC ) / (SH * R * T * VL)
0013            GAMO = (WO * VC ) / (SO * R * T * VL)
0014            WRITE (6,10) GAMH, GAMO
0015         10 FORMAT(/,10X'H2 PART.COEFF. = ',D10.3,10X,'O2 PART.COEFF.=',D10.3)
          C
          C  CALCULATION OF H2 AND O2 CONCENTRATIONS FOR MINIMUM BOILING TIME
          C
0016            EMN = 1.4D1
0017            WRITE (6,20) EMN
0018         20 FORMAT(/5X,'MINIMUM BOILING TIME CALC.--',D10.3,' LBS.DECOMPOSED')
0019            DO 45 I =1,12
0020            CH2(I) = (2.7085D2 + 2D0 * FZR(I) * 3.52916D5 + 2.5178D1 * EMN )
0021            PH2(I) = (CH2(I) * R * T) / VC
0022            CH2(I) = CH2(I) / (VL * (GAMH + 1D0))
0023            CO2(I) = (1.0834D4 + 1.25890D1 * EMN)
0024            PO2(I) = (CO2(I) * R * T)/VC
0025            CO2(I) = (CO2(I) / (VL * (GAMO + 1D0)))
0026         45 WRITE (6,50) FZR(I), CH2(I), PH2(I), CO2(I), PO2(I)
0027         50 FORMAT(/3X,'FRACT.ZR-H2O=',D10.3,3X,'(H2)=',D10.3,'MOLES/LITER',
              X 3X,'PH2=',D10.3,'ATMOS.',3X,'(O2)=',D10.3,'MOLES/LITER',3X,
              Y 'PO2=',D10.3,'ATMOS.')
          C
          C     CALCULATION OF H2 AND O2 CONCENTRATIONS FOR
```

```
              C             MAXIMUM BOILING TIME                                    00000580
              C                                                                     00000590
 0028               EMX = 1.1D2                                                     00000600
 0029               WRITE(6,100)EMX                                                 00000610
 0030           100 FORMAT(//5X,'MAXIMUM BOILING TIME CALC.--',D10.3,'LBS.DECOMPOSED')00000620
 0031               DO 25 I =1,12                                                   00000630
 0032               CH2(I) = (2.7085D2 + 2D0 * FZR(I) * 3.52916D5 + 2.5178D1 * EMX )  00000640
 0033               PH2(I) = (CH2(I) * R * T) / VC                                  00000650
 0034               CH2(I) = CH2(I) / (VL * (GAMH + 1D0))                           00000660
 0035               CO2(I) = (1.0834D4 + 1.2589D1 * EMX)                            00000670
 0036               PO2(I) = (CO2(I) * R * T)/VC                                    00000680
 0037               CO2(I) = (CO2(I) / (VL * (GAMO + 1D0)))                         00000690
 0038            25 WRITE (6,50) FZR(I), CH2(I), PH2(I), CO2(I), PO2(I)             00000700
 0039               STOP                                                            00000710
 0040               END                                                             00000720
```

```
     H2 PART.COEFF. =  0.144D 03         O2 PART.COEFF.= 0.113D 03
   MINIMUM BOILING TIME CALC.-- 0.140E 02 LBS.DECOMPOSED
 FRACT.ZR-H2O= 0.0          (H2)= 0.165D-05MOLES/LITER   PH2= 0.227D-02ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.100D-02    (H2)= 0.352D-05MOLES/LITER   PH2= 0.483D-02ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.200D-02    (H2)= 0.540D-05MOLES/LITER   PH2= 0.740D-02ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.500D-02    (H2)= 0.110D-04MOLES/LITER   PH2= 0.151D-01ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.612D-02    (H2)= 0.131D-04MOLES/LITER   PH2= 0.180D-01ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.700D-02    (H2)= 0.148D-04MOLES/LITER   PH2= 0.202D-01ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.100D-01    (H2)= 0.204D-04MOLES/LITER   PH2= 0.279D-01ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.500D-01    (H2)= 0.952D-04MOLES/LITER   PH2= 0.131D 00ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.100D 00    (H2)= 0.189D-03MOLES/LITER   PH2= 0.259D 00ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.200D 00    (H2)= 0.376D-03MOLES/LITER   PH2= 0.516D 00ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.300D 00    (H2)= 0.563D-03MOLES/LITER   PH2= 0.772D 00ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.
 FRACT.ZR-H2O= 0.500D 00    (H2)= 0.937D-03MOLES/LITER   PH2= 0.129D 01ATMOS.   (O2)= 0.371D-04MOLES/LITER   PO2= 0.400D-01ATMOS.

   MAXIMUM BOILING TIME CALC.-- 0.110E 03LBS.DECOMPOSED
 FRACT.ZR-H2O= 0.0          (H2)= 0.806D-05MOLES/LITER   PH2= 0.111D-01ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.100D-02    (H2)= 0.993D-05MOLES/LITER   PH2= 0.136D-01ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.200D-02    (H2)= 0.118D-04MOLES/LITER   PH2= 0.162D-01ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.500D-02    (H2)= 0.174D-04MOLES/LITER   PH2= 0.239D-01ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.612D-02    (H2)= 0.195D-04MOLES/LITER   PH2= 0.268D-01ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.700D-02    (H2)= 0.212D-04MOLES/LITER   PH2= 0.290D-01ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.100D-01    (H2)= 0.268D-04MOLES/LITER   PH2= 0.367D-01ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.500D-01    (H2)= 0.102D-03MOLES/LITER   PH2= 0.139D 00ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.100D 00    (H2)= 0.195D-03MOLES/LITER   PH2= 0.268D 00ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS.
 FRACT.ZR-H2O= 0.200D 00    (H2)= 0.382D-03MOLES/LITER   PH2= 0.524D 00ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS
 FRACT.ZR-H2O= 0.300D 00    (H2)= 0.569D-03MOLES/LITER   PH2= 0.781D 00ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS
 FRACT.ZR-H2O= 0.500D 00    (H2)= 0.944D-03MOLES/LITER   PH2= 0.129D 01ATMOS.   (O2)= 0.412D-04MOLES/LITER   PO2= 0.444D-01ATMOS
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C
C     CALCULATION OF POST-BOILING PHASE DISSOLVED GAS
C     CONCENTRATIONS IN REACTOR COOLANT WATER AND CONTAINMENT
C                       JOHN BICKEL
C                       JUNE 8, 1982
C
C ***********************************************************************
C
      DIMENSION FZR(12), CH2(12), CO2(12), PH2(12), PO2(12)
      REAL * 8 WH, WO, SH, SO ,VC, VL, R, T, GAMH, GAMO, FZR, MNE,
     X CH2, CO2, PH2, PO2
      DATA FZR /0.D0,1.D-3,2.D-3,5.D-3,6.125D-3, 7.D-3, 1.D-2, 5.D-2,
     X          1.D-1, 2.D-1, 3.D-1, 5.D-1/
C     CALCULATION OF MOLAR PARTITION COEFFICIENTS
C     WX = MOLECULAR WEIGHT IN GRAMS/MOLE
C     SX = SOLUBILITY IN MILLIGRAMS/LITER H2O
C     VC = CONTAINMENT VOLUME IN LITERS
C     VL = LIQUID VOLUME IN LITERS
C     R  = GAS LAW CONSTANT
C     T  = ABSOLUTE TEMPERATURE IN DEGREES KELVIN
C
C ***********************************************************************
      WH = 2.016D0
      WO = 3.19981D1
      SH = 1.535D-3
      SO = 2.585D-2
      VC = 7.291D6
      VL = 2.605D6
      R  = 8.205D-2
      T  = 3.4815D2
      GAMH = (WH * VC ) / (SH * R * T * VL)
      GAMO = (WO * VC ) / (SO * R * T * VL)
      WRITE (6,10) GAMH, GAMO
   10 FORMAT(/,10X'H2 PART.COEFF. = ',D10.3,10X,'O2 PART.COEFF.=',D10.3)
C
C  CALCULATION OF H2 AND O2 CONCENTRATIONS FOR MINIMUM BOILING TIME
C
      EMN = 1.4D1
      WRITE (6,20) EMN
   20 FORMAT(/5X,'MINIMUM BOILING TIME CALC.--',D10.3,' LBS.DECOMPOSED')
      DO 45 I =1,12
      CH2(I) = (2.7085D2 + 2D0 * FZR(I) * 3.52916D5 + 2.5178D1 * EMN )
      PH2(I) = (CH2(I) * R * T) / VC
      CH2(I) = CH2(I) / (VL * (GAMH + 1D0))
      CO2(I) = (1.0834D4 + 1.2589D1 * EMN)
      PO2(I) = (CO2(I) * R * T)/VC
      CO2(I) = (CO2(I) / (VL * (GAMO + 1D0)))
   45 WRITE (6,50) FZR(I), CH2(I), PH2(I), CO2(I), PO2(I)
   50 FORMAT(/3X,'FRACT.ZR-H2O=',D10.3,3X,'(H2)=',D10.3,'MOLES/LITER',
     X 3X,'PH2=',D10.3,'ATMOS.',3X,'(O2)=',D10.3,'MOLES/LITER',3X,
     Y 'PO2=',D10.3,'ATMOS.')
C
C     CALCULATION OF H2 AND O2 CONCENTRATIONS FOR
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CASE III

T=75°C

FIG. F-5

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            C                MAXIMUM BOILING TIME                               00000580
            C                                                                   00000590
 0028             EMX = 1.1D2                                                   00000600
 0029             WRITE(6,100)EMX                                               00000610
 0030         100 FORMAT(//5X,'MAXIMUM BOILING TIME CALC.--',D10.3,'LBS.DECOMPOSED')00000620
 0031             DO 25 I =1,12                                                 00000630
 0032             CH2(I) = (2.7085D2 + 2D0 * FZR(I) * 3.5291605 + 2.5178D1 * EMX )  00000640
 0033             PH2(I) = (CH2(I) * R * T) / VC                                00000650
 0034             CH2(I) = CH2(I) / (VL * (GAMH + 1D0))                         00000660
 0035             CO2(I) = (1.0834D4 + 1.2589D1 * EMX)                          00000670
 0036             PO2(I) = (CO2(I) * R * T)/VC                                  00000680
 0037             CO2(I) = (CO2(I) / (VL * (GAMO + 1D0)))                       00000690
 0038          25 WRITE (6,50) FZR(I), CH2(I), PH2(I), CO2(I), PO2(I)           00000700
 0039             STOP                                                          00000710
 0040             END                                                           00000720
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      H2 PART.COEFF. =  0.129D 03          O2 PART.COEFF.= 0.121D 03

   MINIMUM BOILING TIME CALC.-- 0.140E 02 LBS.DECOMPOSED

  FRACT.ZR-H2O= 0.0          (H2)= 0.185D-05MOLES/LITER   PH2= 0.244D-02ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.100D-02    (H2)= 0.393D-05MOLES/LITER   PH2= 0.521D-02ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.200D-02    (H2)= 0.602D-05MOLES/LITER   PH2= 0.797D-02ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.500D-02    (H2)= 0.123D-04MOLES/LITER   PH2= 0.163D-01ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.612D-02    (H2)= 0.146D-04MOLES/LITER   PH2= 0.194D-01ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.700D-02    (H2)= 0.165D-04MOLES/LITER   PH2= 0.218D-01ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.100D-01    (H2)= 0.227D-04MOLES/LITER   PH2= 0.301D-01ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.500D-01    (H2)= 0.106D-03MOLES/LITER   PH2= 0.141D 00ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.100D 00    (H2)= 0.211D-03MOLES/LITER   PH2= 0.279D 00ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.200D 00    (H2)= 0.420D-03MOLES/LITER   PH2= 0.556D 00ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.300D 00    (H2)= 0.629D-03MOLES/LITER   PH2= 0.832D 00ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

  FRACT.ZR-H2O= 0.500D 00    (H2)= 0.105D-02MOLES/LITER   PH2= 0.139D 01ATMOS.   (O2)= 0.346D-04MOLES/LITER   PO2= 0.431D-01ATMOS.

   MAXIMUM BOILING TIME CALC.-- 0.110E 03LBS.DECOMPOSED

  FRACT.ZR-H2O= 0.0          (H2)= 0.900D-05MOLES/LITER   PH2= 0.119D-01ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.100D-02    (H2)= 0.111D-04MOLES/LITER   PH2= 0.147D-01ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.200D-02    (H2)= 0.132D-04MOLES/LITER   PH2= 0.174D-01ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.500D-02    (H2)= 0.194D-04MOLES/LITER   PH2= 0.257D-01ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.612D-02    (H2)= 0.218D-04MOLES/LITER   PH2= 0.289D-01ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.700D-02    (H2)= 0.236D-04MOLES/LITER   PH2= 0.313D-01ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.100D-01    (H2)= 0.299D-04MOLES/LITER   PH2= 0.396D-01ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.500D-01    (H2)= 0.113D-03MOLES/LITER   PH2= 0.150D 00ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.100D 00    (H2)= 0.218D-03MOLES/LITER   PH2= 0.288D 00ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS.

  FRACT.ZR-H2O= 0.200D 00    (H2)= 0.427D-03MOLES/LITER   PH2= 0.565D 00ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS

  FRACT.ZR-H2O= 0.300D 00    (H2)= 0.636D-03MOLES/LITER   PH2= 0.842D 00ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS

  FRACT.ZR-H2O= 0.500D 00    (H2)= 0.105D-02MOLES/LITER   PH2= 0.139D 01ATMOS.   (O2)= 0.384D-04MOLES/LITER   PO2= 0.479D-01ATMOS
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FORTRAN IV G LEVEL  21                MAIN             DATE = 82165          12/29/48              PAGE 0001
      C
      C     CALCULATION OF POST-BOILING PHASE DISSOLVED GAS
      C     CONCENTRATIONS IN REACTOR COOLANT WATER AND CONTAINMENT
      C                       JOHN BICKEL
      C                       JUNE 8, 1982
      C
      C ******************************************************************
      C
            DIMENSION FZR(12), CH2(12), CO2(12), PH2(12), PO2(12)
            REAL * 8 WH, WO, SH, SO ,VC, VL, R, T, GAMH, GAMO, FZR, MNE,
           X CH2, CO2, PH2, PO2
            DATA FZR /0.D0,1.D-3,2.D-3,5.D-3,6.125D-3, 7.D-3, 1.D-2, 5.D-2,
           X          1.D-1, 2.D-1, 3.D-1, 5.D-1/
      C     CALCULATION OF MOLAR PARTITION COEFFICIENTS
      C     WX = MOLECULAR WEIGHT IN GRAMS/MOLE
      C     SX = SOLUBILITY IN MILLIGRAMS/LITER H2O
      C     VC = CONTAINMENT VOLUME IN LITERS
      C     VL = LIQUID VOLUME IN LITERS
      C     R  = GAS LAW CONSTANT
      C     T  = ABSOLUTE TEMPERATURE IN DEGREES KELVIN
      C
      C ******************************************************************
            WH = 2.016D0
            WO = 3.19981D1
            SH = 1.685D-3
            SO = 2.52D-2
            VC = 7.291D6
            VL = 2.605D6
            R  = 8.205D-2
            T  = 3.7315D2
            GAMH = (WH * VC ) / (SH * R * T * VL)
            GAMO = (WO * VC ) / (SO * R * T * VL)
            WRITE (6,10) GAMH, GAMO
         10 FORMAT(/,10X'H2 PART.COEFF. = ',D10.3,10X,'O2 PART.COEFF.=',D10.3)
      C
      C  CALCULATION OF H2 AND O2 CONCENTRATIONS FOR MINIMUM BOILING TIME
      C
            EMN = 1.4D1
            WRITE (6,20) EMN
         20 FORMAT(/5X,'MINIMUM BOILING TIME CALC.--',D10.3,' LBS.DECOMPOSED')
            DO 45 I =1,12
            CH2(I) = (2.7085D2 + 2D0 * FZR(I) * 3.52916D5 + 2.5178D1 * EMN )
            PH2(I) = (CH2(I) * R * T) / VC
            CH2(I) = CH2(I) / (VL * (GAMH + 1D0))
            CO2(I) = (1.0834D4 + 1.2589D1 * EMN)
            PO2(I) = (CO2(I) * R * T)/VC
            CO2(I) = (CO2(I) / (VL * (GAMO + 1D0)))
         45 WRITE (6,50) FZR(I), CH2(I), PH2(I), CO2(I), PO2(I)
         50 FORMAT(/3X,'FRACT.ZR-H2O=',D10.3,3X,'(H2)=',D10.3,'MOLES/LITER',
           X 3X,'PH2=',D10.3,'ATMOS.',3X,'(O2)=',D10.3,'MOLES/LITER',3X,
           Y 'PO2=',D10.3,'ATMOS.')
      C
      C     CALCULATION OF H2 AND O2 CONCENTRATIONS FOR
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CASE IV

T=100°C

FIG. F-6

```
      C                 MAXIMUM BOILING TIME                                    00000580
      C                                                                         00000590
            EMX = 1.1D2                                                         00000600
            WRITE(6,100)EMX                                                     00000610
        100 FORMAT(//5X,'MAXIMUM BOILING TIME CALC.--',D10.3,'LBS.DECOMPOSED')00000620
            DO 25 I =1,12                                                       00000630
            CH2(I) = (2.7085D2 + 2D0 * FZR(I) * 3.52916D5 + 2.5178D1 * EMX )  00000640
            PH2(I) = (CH2(I) * R * T) / VC                                      00000650
            CH2(I) = CH2(I) / (VL * (GAMH + 1D0))                               00000660
            CO2(I) = (1.0834D4 + 1.2589D1 * EMX)                                00000670
            PO2(I) = (CO2(I) * R * T)/VC                                        00000680
            CO2(I) = (CO2(I) / (VL * (GAMO + 1D0)))                             00000690
         25 WRITE (6,50) FZR(I), CH2(I), PH2(I), CO2(I), PO2(I)                 00000700
            STOP                                                                00000710
            END                                                                 00000720
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      H2 PART.COEFF. =  0.109D 03          O2 PART.COEFF.= 0.116D 03

   MINIMUM BOILING TIME CALC.-- 0.140E 02 LBS.DECOMPOSED

  FRACT.ZR-H2O= 0.0          (H2)= 0.217D-05MOLES/LITER   PH2= 0.262D-02ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.100D-02    (H2)= 0.462D-05MOLES/LITER   PH2= 0.558D-02ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.200D-02    (H2)= 0.708D-05MOLES/LITER   PH2= 0.855D-02ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.500D-02    (H2)= 0.144D-04MOLES/LITER   PH2= 0.174D-01ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.612D-02    (H2)= 0.172D-04MOLES/LITER   PH2= 0.208D-01ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.700D-02    (H2)= 0.194D-04MOLES/LITER   PH2= 0.234D-01ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.100D-01    (H2)= 0.267D-04MOLES/LITER   PH2= 0.323D-01ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.500D-01    (H2)= 0.125D-03MOLES/LITER   PH2= 0.151D 00ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.100D 00    (H2)= 0.248D-03MOLES/LITER   PH2= 0.299D 00ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.200D 00    (H2)= 0.493D-03MOLES/LITER   PH2= 0.595D 00ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.300D 00    (H2)= 0.739D-03MOLES/LITER   PH2= 0.892D 00ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.
  FRACT.ZR-H2O= 0.500D 00    (H2)= 0.123D-02MOLES/LITER   PH2= 0.148D 01ATMOS.   (O2)= 0.361D-04MOLES/LITER   PO2= 0.462D-01ATMOS.

   MAXIMUM BOILING TIME CALC.-- 0.110E 03LBS.DECOMPOSED

  FRACT.ZR-H2O= 0.0          (H2)= 0.106D-04MOLES/LITER   PH2= 0.128D-01ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.100D-02    (H2)= 0.130D-04MOLES/LITER   PH2= 0.157D-01ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.200D-02    (H2)= 0.155D-04MOLES/LITER   PH2= 0.187D-01ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.500D-02    (H2)= 0.228D-04MOLES/LITER   PH2= 0.276D-01ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.612D-02    (H2)= 0.256D-04MOLES/LITER   PH2= 0.309D-01ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.700D-02    (H2)= 0.278D-04MOLES/LITER   PH2= 0.335D-01ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.100D-01    (H2)= 0.351D-04MOLES/LITER   PH2= 0.424D-01ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.500D-01    (H2)= 0.133D-03MOLES/LITER   PH2= 0.161D 00ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.100D 00    (H2)= 0.256D-03MOLES/LITER   PH2= 0.309D 00ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.200D 00    (H2)= 0.502D-03MOLES/LITER   PH2= 0.606D 00ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.300D 00    (H2)= 0.747D-03MOLES/LITER   PH2= 0.902D 00ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
  FRACT.ZR-H2O= 0.500D 00    (H2)= 0.124D-02MOLES/LITER   PH2= 0.149D 01ATMOS.   (O2)= 0.401D-04MOLES/LITER   PO2= 0.513D-01ATMOS.
```

APPENDIX G

HYDROGEN AND OXYGEN GAS TRANSPORT RATE

SENSITIVITY ANALYSIS

This appendix documents the results of the sensitivity analysis of the BASE CASE results to the assumed Gas Transport Rate constants for molecular hydrogen and oxygen gas (from the containment gas volume to the torus liquid volume). Evaluation of this sensitivity is necessitated due to the fact that no ward experimental data exists for these rate constants.

Throughout all of these calculations, the rate constant for gas transport from the containment gas volume to the liquid volume $k_T(X)$ is chosen such that:

$$k_T(H_2) = \sqrt{\frac{m_{O_2}}{m_{H_2}}}\, k_T(O_2) \cong 4.0\, k_T(O_2) \qquad \text{(G-1)}$$

This assures that the rates correspond to those obtainable from gas kinetic theorty. The reverse rates (transport from liquid to gas volume) or $k_T(X)$, are defined as:

$$k_R(H_2) = \frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)\frac{m_{H_2} k_T(H_2)}{S_{H_2}} \qquad \text{(G-2)}$$

$$k_R(O_2) = \frac{1}{RT}\left(\frac{V_{cont}}{V_{torus}}\right)\frac{m_{O_2} k_T(O_2)}{S_{O_2}} \qquad \text{(G-3)}$$

Use of these values assure equilibrium partitioning according to Henry's Law.

Three typical examples are shown using input data defined below:

Simulation	Figure	Assumptions
CASE I	Fig. G-1	$k_T(H_2) = 4.0$ $k_T(O_2) = 1.0$
CAST II	Fig. G-2	$k_T(H_2) = 40.0$ $k_T(O_2) = 10.0$
CAST III	Fig. G-3	$k_T(H_2) = 0.4$ $k_T(O_2) = 0.1$

- All other inputs are as assumed in Figure XVII of Section 4.2 in Vol. I.

It is anticipated that the impact of the specific choice of $k_T(X)$ values will only affect the dynamics in time frame of <10 seconds, but will have no effect on long term simulations which are of greater concern.

Key Parameters Printed Out Include:

DOMR	Accumulated dose in Megarads
TIME	Time in units of seconds
H_2O_2	Molecular, ionic, and radical species in Moles/Liter within the core region

H^+	Molecular, ionic, and radical species in Moles/Liter within the core region
OH^-	Molecular, ionic, and radical species in Moles/Liter within the core region
O_2-	Molecular, ionic, and radical species in Moles/Liter within the core region
H	Molecular, ionic, and radical species in Moles/Liter within the core region
OH	Molecular, ionic, and radical species in Moles/Liter within the core region
E^-	Molecular, ionic, and radical species in Moles/Liter within the core region
HO_2	Molecular, ionic, and radical species in Moles/Liter within the core region
HO_2-	Molecular, ionic, and radical species in Moles/Liter within the core region
H_2	Molecular, ionic, and radical species in Moles/Liter within the core region

O_2	Molecular, ionic, and radical species in Moles/Liter within the core region
H2T O2T H2O2T	Scaled molecular species in Moles/Liter within the Torus, $H2T = [H_2]_T(V_{torus}/V_{core})$ etc.

```
PRINT STREAM NO.  2
  DOMR        H2O2        H+          OH-         PSO2        O2-         H           OH          PSH2        E-
  2.1789D-03  3.8375D-06  1.7854D-07  5.6037D-08  4.1000D-02  1.2247D-07  3.5029D-13  2.1988D-10  3.3900D-02  5.2933D-13
  2.1782D-02  1.9552D-05  1.7535D-07  5.7040D-08  4.0998D-02  1.1811D-07  4.0055D-13  2.4035D-10  3.3899D-02  5.3142D-13
  2.1718D-01  2.1536D-05  1.7170D-07  5.8249D-08  4.0968D-02  1.1323D-07  3.7288D-13  2.6257D-10  3.3876D-02  5.3784D-13
  2.1181D+00  2.9433D-05  1.7458D-07  5.7276D-08  4.0757D-02  1.1701D-07  2.9232D-13  2.2500D-10  3.3651D-02  4.1037D-13
  1.8621D+01  3.2740D-05  1.6884D-07  5.9215D-08  3.9756D-02  1.0928D-07  2.2507D-13  1.8109D-10  3.1717D-02  3.0817D-13
  1.2095D+02  2.8505D-05  1.5050D-07  6.6437D-08  3.3888D-02  8.3729D-08  1.3455D-13  1.2403D-10  1.9887D-02  1.9155D-13
  5.1569D+02  2.2559D-05  1.2675D-07  7.8896D-08  2.8101D-02  4.7545D-08  3.9746D-14  5.2360D-11  8.2006D-03  6.3545D-14
  9.9111D+02  2.1328D-05  1.0776D-07  9.2805D-08  2.6692D-02  1.4605D-08  2.7698D-15  5.2259D-12  5.3566D-03  4.4549D-15
```

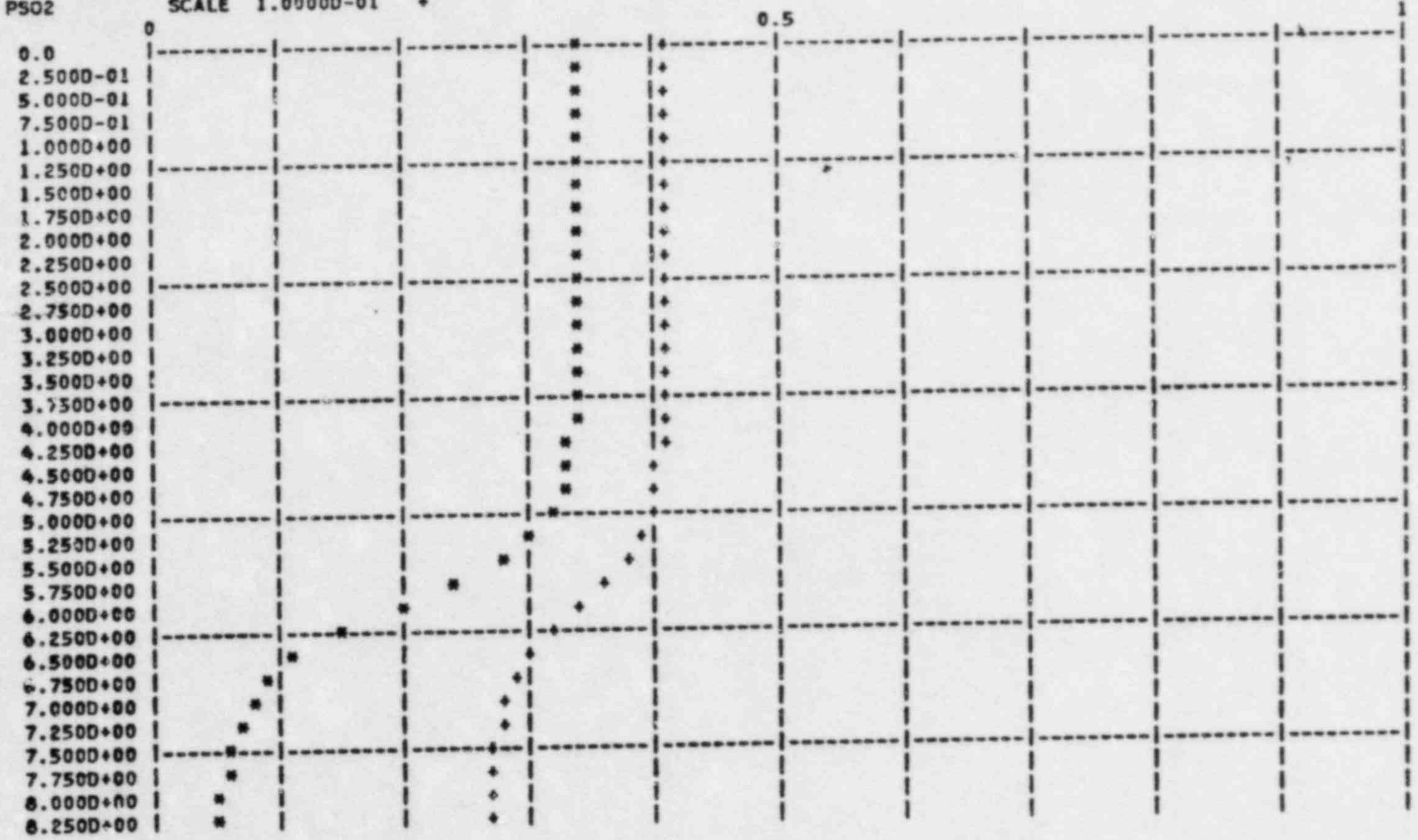
FIG. G-1

```
PRINT STREAM NO.  3
  DOMR         HO2          H2O          HO2-         PO2          PH2          PSO2         PSH2
  2.17890-03   1.36700-09   5.53000+01   3.78170-11   4.55030-02   3.76230-02   4.10000-02   3.39000-02
  2.17820-02   1.29500-09   5.53000+01   1.96120-10   4.55010-02   3.76220-02   4.09980-02   3.38990-02
  2.17180-01   1.21560-09   5.53000+01   2.20620-10   4.54670-02   3.75970-02   4.09680-02   3.38760-02
  2.11810+00   1.27730-09   5.53000+01   2.96460-10   4.52330-02   3.73470-02   4.07570-02   3.36510-02
  1.86210+01   1.15370-09   5.53020+01   3.40930-10   4.41230-02   3.52010-02   3.97560-02   3.17170-02
  1.20950+02   7.87810-10   5.53150+01   3.33220-10   3.76100-02   2.20710-02   3.38880-02   1.98870-02
  5.15690+02   3.76740-10   5.53280+01   3.13360-10   3.11870-02   9.10120-03   2.81010-02   8.20060-03
  9.91110+02   9.83710-11   5.53320+01   3.48690-10   2.96230-02   5.94490-03   2.66920-02   5.35660-03
```

```
PRINT STREAM NO.  4
  DOMR        TIME        H2T         O2T         H2O2T
  2.1789D-03  1.0000D+01  2.5775D-04  5.0473D-04  4.6287D-08
  2.1782D-02  1.0000D+02  2.5774D-04  5.0468D-04  2.9628D-06
  2.1718D-01  1.0000D+03  2.5756D-04  5.0430D-04  4.3200D-05
  2.1181D+00  1.0000D+04  2.5585D-04  5.0172D-04  2.4368D-04
  1.8621D+01  1.0000D+05  2.4115D-04  4.8941D-04  3.2095D-04
  1.2095D+02  1.0000D+06  1.5120D-04  4.1718D-04  2.7953D-04
  5.1569D+02  1.0000D+07  6.2353D-05  3.4594D-04  2.2110D-04
  9.9111D+02  1.0000D+08  4.0728D-05  3.2859D-04  2.0902D-04
```

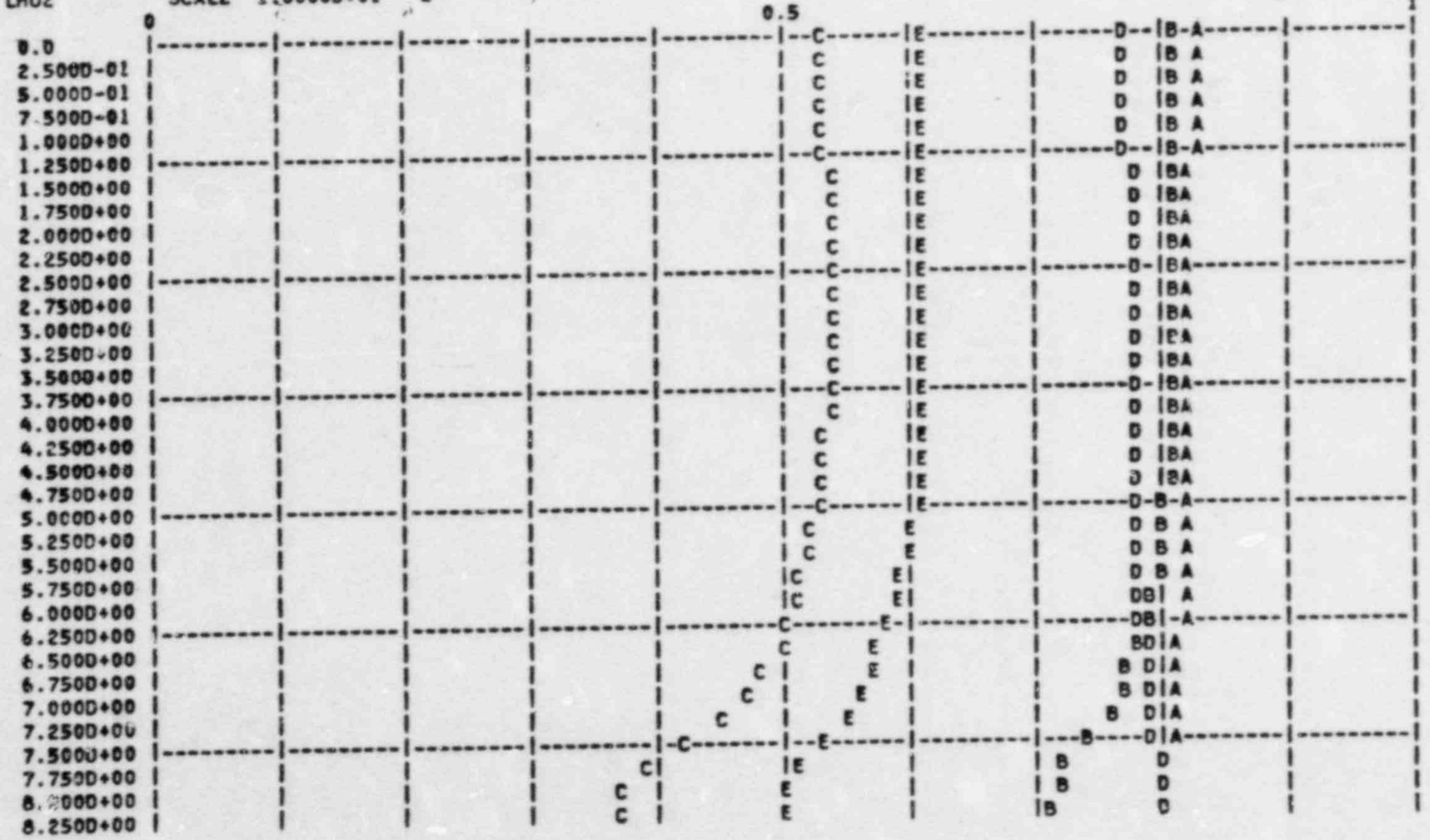
```
PRINT STREAM NO.  6
  DOMR         H2O2         H+           OH-          O2           O2-          H            OH           H2           E-
  LH2          LO2          LH2O2        LH+          LO2-         LOH          LHO2         LE-          LH           LHO2-
  2.1789D-03   3.8375D-06   1.7854D-07   5.6037D-08   4.8972D-05   1.2247D-07   3.5029D-13   2.1988D-10   2.5263D-05   5.2933D-13
  1.0402D+01   1.0690D+01   9.5841D+00   8.2517D+00   8.0880D+00   5.3422D+00   6.1358D+00   2.7237D+00   2.5444D+00   4.5777D+00
  2.1782D-02   1.9552D-05   1.7535D-07   5.7040D-08   3.7988D-05   1.1811D-07   4.0055D-13   2.4035D-10   1.8945D-05   5.3142D-13
  1.0278D+01   1.0580D+01   1.0291D+01   8.2439D+00   8.0723D+00   5.3808D+00   6.1123D+00   2.7254D+00   2.6027D+00   5.2925D+00
  2.1718D-01   2.1536D-05   1.7170D-07   5.8249D-08   3.5722D-05   1.1323D-07   3.7288D-13   2.6257D-10   1.3600D-05   5.3784D-13
  1.0134D+01   1.0553D+01   1.0333D+01   8.2348D+00   8.0540D+00   5.4192D+00   6.0848D+00   2.7307D+00   2.5716D+00   5.3437D+00
  2.1181D+00   2.9433D-05   1.7458D-07   5.7276D-08   4.3065D-05   1.1701D-07   2.9232D-13   2.2500D-10   1.4906D-05   4.1037D-13
  1.0173D+01   1.0634D+01   1.0469D+01   8.2420D+00   8.0682D+00   5.3522D+00   6.1063D+00   2.6132D+00   2.4659D+00   5.4720D+00
  1.8621D+01   3.2740D-05   1.6884D-07   5.9215D-08   4.5176D-05   1.0928D-07   2.2507D-13   1.8109D-10   1.5072D-05   3.0817D-13
  1.0178D+01   1.0655D+01   1.0515D+01   8.2275D+00   8.0386D+00   5.2579D+00   6.0621D+00   2.4888D+00   2.3523D+00   5.5327D+00
  1.2095D+02   2.8505D-05   1.5050D-07   6.6437D-08   4.0598D-05   8.3729D-08   1.3455D-13   1.2403D-10   1.1470D-05   1.9155D-13
  1.0060D+01   1.0609D+01   1.0455D+01   8.1775D+00   7.9229D+00   5.0935D+00   5.8964D+00   2.2823D+00   2.1289D+00   5.5227D+00
  5.1569D+02   2.2559D-05   1.2675D-07   7.8896D-08   3.5265D-05   4.7545D-08   3.9746D-14   5.2360D-11   6.2954D-06   6.3545D-14
  9.7990D+00   1.0547D+01   1.0353D+01   8.1030D+00   7.6771D+00   4.7190D+00   5.5760D+00   1.8031D+00   1.5993D+00   5.4960D+00
  9.9111D+02   2.1328D-05   1.0776D-07   9.2805D-08   3.3527D-05   1.4605D-08   2.7698D-15   5.2259D-12   4.1545D-06   4.4549D-15
  9.6185D+00   1.0525D+01   1.0329D+01   8.0325D+00   7.1645D+00   3.7182D+00   4.9929D+00   6.4883D-01   4.4244D-01   5.5424D+00
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2          SCALE  1.0000D-01   *
PSO2          SCALE  1.0000D-01   +
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2          SCALE  2.0000D+01   A
LO2          SCALE  2.0000D+01   B
LH2O2        SCALE  2.0000D+01   C
           0                                                0.5                                               1
0.0        |---------|---------|---------|---------|--C------|-A-B-----|---------|---------|---------|---------|
2.5000D-01 |         |         |         |         |   C     | A B     |         |         |         |         |
5.0000D-01 |         |         |         |         |    C    | A B     |         |         |         |         |
7.5000D-01 |         |         |         |         |      C  | AB      |         |         |         |         |
1.0000D+00 |         |         |         |         |       C | AB      |         |         |         |         |
1.2500D+00 |---------|---------|---------|---------|--------C|-AB------|---------|---------|---------|---------|
1.5000D+00 |         |         |         |         |         C AB      |         |         |         |         |
1.7500D+00 |         |         |         |         |         |CAB      |         |         |         |         |
2.0000D+00 |         |         |         |         |         |C B      |         |         |         |         |
2.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
2.5000D+00 |---------|---------|---------|---------|---------|ACB------|---------|---------|---------|---------|
2.7500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
3.0000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
3.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
3.5000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
3.7500D+00 |---------|---------|---------|---------|---------|ACB------|---------|---------|---------|---------|
4.0000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
4.2500D+00 |         |         |         |         |         |A C      |         |         |         |         |
4.5000D+00 |         |         |         |         |         |A C      |         |         |         |         |
4.7500D+00 |         |         |         |         |         |A C      |         |         |         |         |
5.0000D+00 |---------|---------|---------|---------|---------|A-C------|---------|---------|---------|---------|
5.2500D+00 |         |         |         |         |         |A C      |         |         |         |         |
5.5000D+00 |         |         |         |         |         |A C      |         |         |         |         |
5.7500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
6.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
6.2500D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
6.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
6.7500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.0000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.2500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.5000D+00 |---------|---------|---------|---------|-------A-|-CB------|---------|---------|---------|---------|
7.7500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
8.0000D+00 |         |         |         |         |       A | CB      |         |         |         |         |
8.2500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 13
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+           SCALE  1.00000D+01    A
LO2-          SCALE  1.00000D+01    B
LOH           SCALE  1.00000D+01    C
LOH-          SCALE  1.00000D+01    D
LHO2          SCALE  1.00000D+01    E
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM 11
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-            SCALE  1.00000D+01   A
LH             SCALE  1.00000D+01   B
LHO2-          SCALE  1.00000D+01   C
           0        .1        .2        .3        .4        0.5
 0.0       |---------|---------|----B-A--|-----C---|---------|---------|---------|---------|---------|---------|
 2.500D-01 |         |         |    B A  |       C |         |         |         |         |         |         |
 5.000D-01 |         |         |    B A  |         |C        |         |         |         |         |         |
 7.500D-01 |         |         |    B A  |         |  C      |         |         |         |         |         |
 1.000D+00 |         |         |    B A  |         |     C   |         |         |         |         |         |
 1.250D+00 |---------|---------|-----BA--|---------|-------C-|---------|---------|---------|---------|---------|
 1.500D+00 |         |         |     BA  |         |         C         |         |         |         |         |
 1.750D+00 |         |         |     BA  |         |         | C       |         |         |         |         |
 2.000D+00 |         |         |     BA  |         |         |  C      |         |         |         |         |
 2.250D+00 |         |         |     BA  |         |         |  C      |         |         |         |         |
 2.500D+00 |---------|---------|-----BA--|---------|---------|--C------|---------|---------|---------|---------|
 2.750D+00 |         |         |     BA  |         |         |  C      |         |         |         |         |
 3.000D+00 |         |         |     BA  |         |         |  C      |         |         |         |         |
 3.250D+00 |         |         |     BA  |         |         |   C     |         |         |         |         |
 3.500D+00 |         |         |    B A  |         |         |   C     |         |         |         |         |
 3.750D+00 |---------|---------|----B-A--|---------|---------|---C-----|---------|---------|---------|---------|
 4.000D+00 |         |         |    BA   |         |         |    C    |         |         |         |         |
 4.250D+00 |         |         |   B A   |         |         |    C    |         |         |         |         |
 4.500D+00 |         |         |   B A   |         |         |    C    |         |         |         |         |
 4.750D+00 |         |         |   BA    |         |         |    C    |         |         |         |         |
 5.000D+00 |---------|---------|---BA----|---------|---------|----C----|---------|---------|---------|---------|
 5.250D+00 |         |         |  BA     |         |         |    C    |         |         |         |         |
 5.500D+00 |         |         | B A     |         |         |    C    |         |         |         |         |
 5.750D+00 |         |         | BA      |         |         |    C    |         |         |         |         |
 6.000D+00 |         |         |B A      |         |         |    C    |         |         |         |         |
 6.250D+00 |---------|---------B-A-------|---------|---------|----C----|---------|---------|---------|---------|
 6.500D+00 |         |        B|A        |         |         |    C    |         |         |         |         |
 6.750D+00 |         |       B A         |         |         |    C    |         |         |         |         |
 7.000D+00 |         |     B A |         |         |         |    C    |         |         |         |         |
 7.250D+00 |         |   B A   |         |         |         |    C    |         |         |         |         |
 7.500D+00 |---------B-A-------|---------|---------|---------|----C----|---------|---------|---------|---------|
 7.750D+00 |     B A |         |         |         |         |    C    |         |         |         |         |
 8.000D+00 |   B A   |         |         |         |         |    C    |         |         |         |         |
 8.250D+00 |   B A   |         |         |         |         |    C    |         |         |         |         |
```

```
PRINT STREAM NO.  2
  DOMR       H2O2       H+         OH-        P[illegible]O2       O2-        H          OH         PSH2       E-
  2.1789D-03 3.8375D-06 1.7854D-07 5.6037D-08 4.[illegible]000D-02 1.2247D-07 3.5029D-13 2.1988D-10 3.3900D-02 5.29[illegible]-13
  2.1782D-02 1.9552D-05 1.7535D-07 5.7040D-08 4.0998D-02 1.1811D-07 4.0055D-13 2.4035D-10 3.3899D-02 5.3[illegible] 13
  2.1718D-01 2.1537D-05 1.7170D-07 5.8249D-08 4.0968D-02 1.1323D-07 3.7286D-13 2.6256D-10 3.3876D-02 5.[illegible] 13
  2.1181D+00 2.9434D-05 1.7458D-07 5.7276D-08 4.0757D-02 1.1701D-07 2.9232D-13 2.2500D-10 3.3651D-02 4.1[illegible]3
  1.8621D+01 3.2741D-05 1.6884D-07 5.9215D-08 3.9756D-02 1.0928D-07 2.2507D-13 1.8109D-10 3.1717D-02 3.081[illegible]3
  1.2095D+02 2.8505D-05 1.5050D-07 6.6437D-08 3.3888D-02 8.3729D-08 1.3455D-13 1.2403D-10 1.9886D-02 1.9155[illegible]3
  5.1569D+02 2.2559D-05 1.2675D-07 7.8896D-08 2.8101D-02 4.7545D-08 3.9746D-14 5.2360D-11 8.2006D-03 6.3543D-14
  9.9111D+02 2.1328D-05 1.0776D-07 9.2805D-08 2.6692D-02 1.4605D-08 2.7698D-15 5.2259D-12 5.3566D-03 4.4549D-15
```

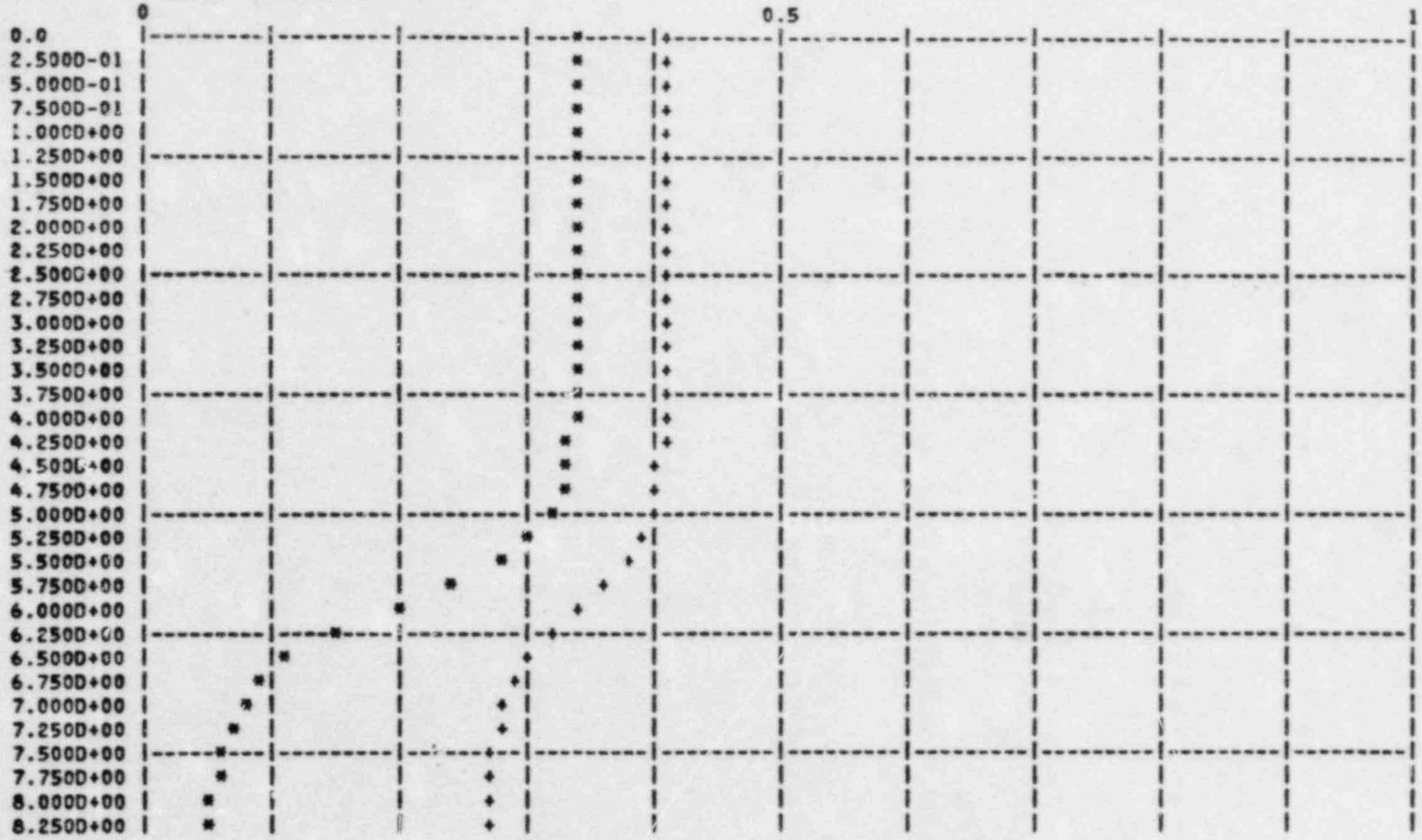
FIG. G-2

```
PRINT STREAM NO.  3
  DOMR         HO2          H2O          HO2-         PO2          PH2          PSO2         PSH2
  2.1789D-03  1.3670D-09  5.5300D+01  3.7817D-11  4.5503D-02  3.7623D-02  4.1000D-02  3.3900D-02
  2.1782D-02  1.2950D-09  5.5300D+01  1.9612D-10  4.5501D-02  3.7622D-02  4.0998D-02  3.3899D-02
  2.1718D-01  1.2156D-09  5.5300D+01  2.2063D-10  4.5467D-02  3.7597D-02  4.0968D-02  3.3876D-02
  2.1181D+00  1.2773D-09  5.5300D+01  2.9647D-10  4.5233D-02  3.7347D-02  4.0757D-02  3.3651D-02
  1.8621D+01  1.1537D-09  5.5302D+01  3.4099D-10  4.4122D-02  3.5201D-02  3.9756D-02  3.1717D-02
  1.2095D+02  7.8781D-10  5.5315D+01  3.3322D-10  3.7610D-02  2.2070D-02  3.3888D-02  1.9886D-02
  5.1569D+02  3.7674D-10  5.5328D+01  3.1336D-10  3.1187D-02  9.1012D-03  2.8101D-02  8.2006D-03
  9.9111D+02  9.8371D-11  5.5332D+01  3.4869D-10  2.9623D-02  5.9449D-03  2.6692D-02  5.3566D-03
```

```
PRINT STREAM NO.  4
  DOMR          TIME          H2T           O2T           H2O2T
  2.1789D-03  1.0000D+01  2.5776D-04  5.0473D-04  4.6287D-08
  2.1782D-02  1.0000D+02  2.5775D-04  5.0471D-04  2.9628D-06
  2.1718D-01  1.0000D+03  2.5757D-04  5.0433D-04  4.3201D-05
  2.1181D+00  1.0000D+04  2.5586D-04  5.0173D-04  2.4369D-04
  1.8621D+01  1.0000D+05  2.4116D-04  4.8942D-04  3.2096D-04
  1.2095D+02  1.0000D+06  1.5120D-04  4.1718D-04  2.7953D-04
  5.1569D+02  1.0000D+07  6.2353D-05  3.4594D-04  2.2110D-04
  9.9111D+02  1.0000D+08  4.0728D-05  3.2859D-04  2.0902D-04
```

```
PRINT STREAM NO.  6
  DOMR        H2O2        H+          OH-         O2          O2-         H           OH          H2          E-
  LH2         LO2         LH2O2       LH+         LO2-        LOH         LHO2        LE-         LH          LHO2-
  2.1789D-03  3.8375D-06  1.7854D-07  5.6037D-08  4.8972D-05  1.2247D-07  3.5029D-13  2.1988D-10  2.5263D-05  5.2933D-13
  1.0402D+01  1.0690D+01  9.5841D+00  8.2517D+00  8.0880D+00  5.3422D+00  6.1358D+00  2.7237D+00  2.5444D+00  4.5777D+00
  2.1782D-02  1.9552D-05  1.7535D-07  5.7040D-08  3.7989D-05  1.1811D-07  4.0055D-13  2.4035D-10  1.8946D-05  5.3142D-13
  1.0278D+01  1.0580D+01  1.0291D+01  8.2439D+00  8.0723D+00  5.3808D+00  6.1123D+00  2.7254D+00  2.6027D+00  5.2925D+00
  2.1718D-01  2.1537D-05  1.7170D-07  5.8249D-08  3.5724D-05  1.1323D-07  3.7286D-13  2.6256D-10  1.3601D-05  5.3781D-13
  1.0134D+01  1.0553D+01  1.0333D+01  8.2348D+00  8.0540D+00  5.4192D+00  6.0848D+00  2.7306D+00  2.5715D+00  5.3437D+00
  2.1181D+00  2.9434D-05  1.7458D-07  5.7276D-08  4.3067D-05  1.1701D-07  2.9230D-13  2.2500D-10  1.4907D-05  4.1036D-13
  1.0173D+01  1.0634D+01  1.0469D+01  8.2420D+00  8.0682D+00  5.3522D+00  6.1063D+00  2.6132D+00  2.4659D+00  5.4720D+00
  1.8621D+01  3.2741D-05  1.6884D-07  5.9215D-08  4.5177D-05  1.0928D-07  2.2507D-13  1.8109D-10  1.5072D-05  3.0816D-13
  1.0178D+01  1.0655D+01  1.0515D+01  8.2275D+00  8.0386D+00  5.2579D+00  6.0621D+00  2.4888D+00  2.3523D+00  5.5327D+00
  1.2095D+02  2.8505D-05  1.5050D-07  6.6437D-08  4.0598D-05  8.3729D-08  1.3455D-13  1.2403D-10  1.1470D-05  1.9155D-13
  1.0060D+01  1.0609D+01  1.0455D+01  8.1775D+00  7.9229D+00  5.0935D+00  5.8964D+00  2.2823D+00  2.1289D+00  5.5227D+00
  5.1569D+02  2.2559D-05  1.2675D-07  7.8896D-08  3.5265D-05  4.7545D-08  3.9746D-14  5.2360D-11  6.2954D-06  6.3545D-14
  9.7990D+00  1.0547D+01  1.0353D+01  8.1030D+00  7.6771D+00  4.7190D+00  5.5760D+00  1.8031D+00  1.5993D+00  5.4960D+00
  9.9111D+02  2.1328D-05  1.0776D-07  9.2805D-08  3.3527D-05  1.4605D-08  2.7698D-15  5.2259D-12  4.1545D-06  4.4549D-15
  9.6185D+00  1.0525D+01  1.0329D+01  8.0325D+00  7.1645D+00  3.7182D+00  4.9929D+00  6.4883D-01  4.4244D-01  5.5424D+00
```

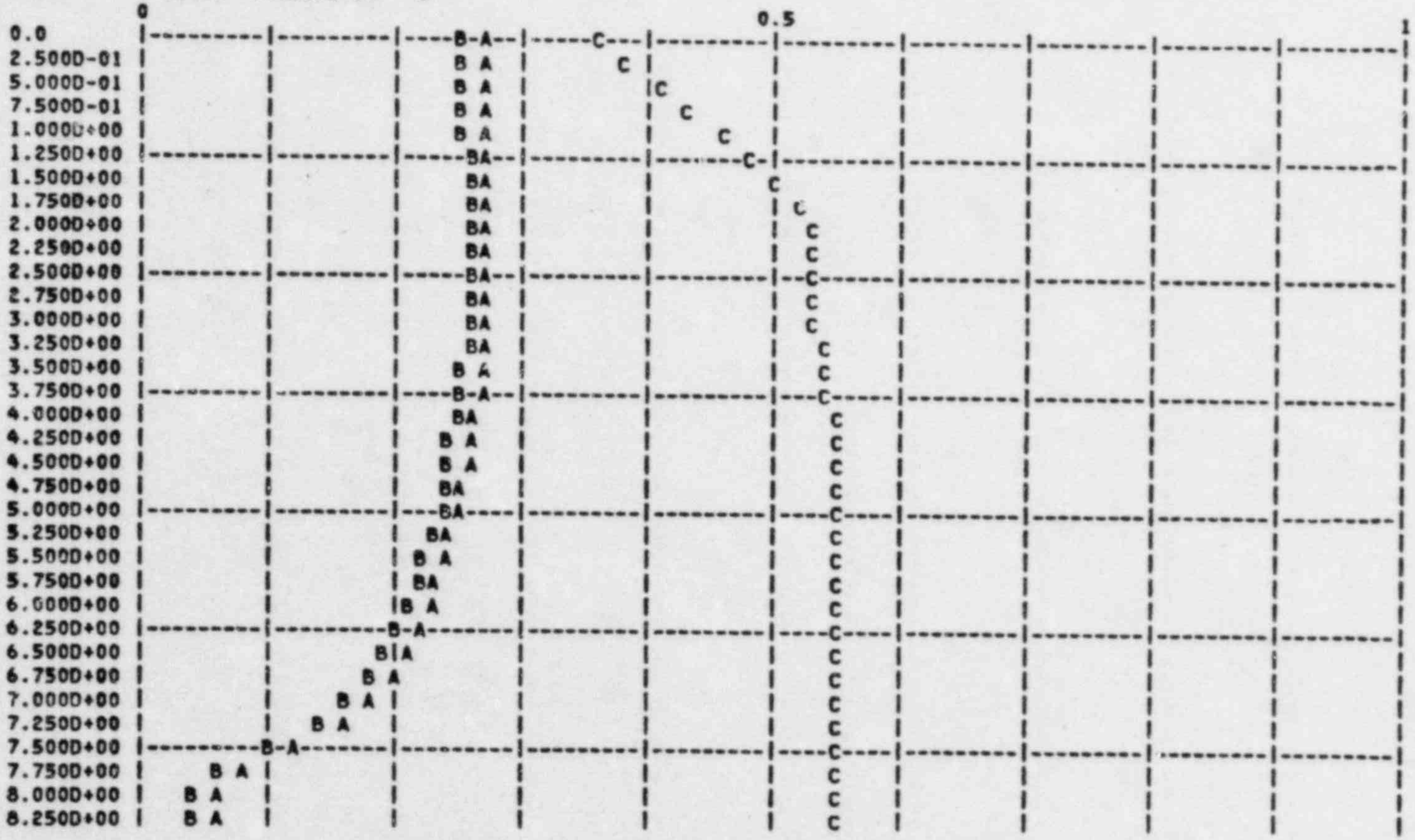
```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2          SCALE  1.0000D-01    *
PSO2          SCALE  1.0000D-01    +
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2          SCALE  2.0000D+01   A
LO2          SCALE  2.0000D+01   B
LH2O2        SCALE  2.0000D+01   C
           0                                                0.5                                                1
0.0        |---------|---------|---------|---------|--C------|-A-B-----|---------|---------|---------|---------|
2.5000D-01 |         |         |         |         |   C     | A B     |         |         |         |         |
5.0000D-01 |         |         |         |         |    C    | A B     |         |         |         |         |
7.5000D-01 |         |         |         |         |      C  | AB      |         |         |         |         |
1.0000D+00 |         |         |         |         |       C | AB      |         |         |         |         |
1.2500D+00 |---------|---------|---------|---------|--------C|-AB------|---------|---------|---------|---------|
1.5000D+00 |         |         |         |         |         C AB      |         |         |         |         |
1.7500D+00 |         |         |         |         |         |CAB      |         |         |         |         |
2.0000D+00 |         |         |         |         |         |C B      |         |         |         |         |
2.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
2.5000D+00 |---------|---------|---------|---------|---------|ACB------|---------|---------|---------|---------|
2.7500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
3.0000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
3.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
3.5000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
3.7500D+00 |---------|---------|---------|---------|---------|ACB------|---------|---------|---------|---------|
4.0000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
4.2500D+00 |         |         |         |         |         |A C      |         |         |         |         |
4.5000D+00 |         |         |         |         |         |A C      |         |         |         |         |
4.7500D+00 |         |         |         |         |         |A C      |         |         |         |         |
5.0000D+00 |---------|---------|---------|---------|---------|A-C------|---------|---------|---------|---------|
5.2500D+00 |         |         |         |         |         |A C      |         |         |         |         |
5.5000D+00 |         |         |         |         |         |A C      |         |         |         |         |
5.7500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
6.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
6.2500D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
6.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
6.7500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.0000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.2500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.5000D+00 |---------|---------|---------|---------|-------A-|-CB------|---------|---------|---------|---------|
7.7500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
8.0000D+00 |         |         |         |         |       A | CB      |         |         |         |         |
8.2500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 10
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+           SCALE  1.0000D+01   A
LO2-          SCALE  1.0000D+01   B
LOH           SCALE  1.0000D+01   C
LOH-          SCALE  1.0000D+01   D
LHO2          SCALE  1.0000D+01   E
           0                                                0.5                                                1
 0.0       |---------|---------|---------|---------|---------|--C------|E--------|------D--|B-A------|---------|
2.5000D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
5.0000D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
7.5000D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
1.0000D+00 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
1.2500D+00 |---------|---------|---------|---------|---------|--C------|E--------|------D--|B-A------|---------|
1.5000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
1.7500D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
2.0000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
2.2500D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
2.5000D+00 |---------|---------|---------|---------|---------|---C-----|E--------|-------D-|BA-------|---------|
2.7500D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
3.0000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
3.2500D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
3.5000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
3.7500D+00 |---------|---------|---------|---------|---------|---C-----|E--------|-------D-|BA-------|---------|
4.0000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
4.2500D+00 |         |         |         |         |         |  C      |E        |       D |BA       |         |
4.5000D+00 |         |         |         |         |         |  C      |E        |       D |BA       |         |
4.7500D+00 |         |         |         |         |         |  C      |E        |       D |BA       |         |
5.0000D+00 |---------|---------|---------|---------|---------|--C------|E--------|-------D-B-A-------|---------|
5.2500D+00 |         |         |         |         |         | C       E         |       D B A       |         |
5.5000D+00 |         |         |         |         |         | C       E         |       D B A       |         |
5.7500D+00 |         |         |         |         |         |C       E|         |       D B A       |         |
6.0000D+00 |         |         |         |         |         |C       E|         |       DB| A       |         |
6.2500D+00 |---------|---------|---------|---------|---------C-------E-|---------|-------DB|-A-------|---------|
6.5000D+00 |         |         |         |         |         C      E  |         |       BD|A        |         |
6.7500D+00 |         |         |         |         |       C |      E  |         |      B D|A        |         |
7.0000D+00 |         |         |         |         |      C  |     E   |         |      B D|A        |         |
7.2500D+00 |         |         |         |         |    C    |    E    |         |     B  D|A        |         |
7.5000D+00 |---------|---------|---------|---------|-C-------|--E------|---------|---B----D|A--------|---------|
7.7500D+00 |         |         |         |        C|         |E        |         | B       D         |         |
8.0000D+00 |         |         |         |      C  |         E         |         | B       D         |         |
8.2500D+00 |         |         |         |      C  |         E         |         |B        D         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 11
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-          SCALE  1.0000D+01   A
LH           SCALE  1.0000D+01   B
LHO2-        SCALE  1.0000D+01   C
```



```
PRINT STREAM NO.  2
  DOMR        H2O2        H+          OH-         PSO2        O2-         H           OH          PSH2        E-
  2.1789D-03  3.8375D-06  1.7854D-07  5.6037D-08  4.1000D-02  1.2247D-07  3.5029D-13  2.1988D-10  3.3900D-02  5.2933D-13
  2.1782D-02  1.9552D-05  1.7535D-07  5.7040D-08  4.0998D-02  1.1811D-07  4.0058D-13  2.4036D-10  3.3899D-02  5.3146D-13
  2.1718D-01  2.1524D-05  1.7169D-07  5.8253D-08  4.0960D-02  1.1321D-07  3.7314D-13  2.6065D-10  3.3876D-02  5.3819D-13
  2.1181D+00  2.9421D-05  1.7457D-07  5.7279D-08  4.0757D-02  1.1700D-07  2.9243D-13  2.2505D-10  3.3651D-02  4.1053D-13
  1.8621D+01  3.2733D-05  1.6834D-07  5.9216D-08  3.9757D-02  1.0928D-07  2.2511D-13  1.8111D-10  3.1718D-02  3.0823D-13
  1.2095D+02  2.8503D-05  1.5050D-07  6.6437D-08  3.3889D-02  8.3728D-08  1.3456D-13  1.2403D-10  1.9888D-02  1.9156D-13
  5.1569D+02  2.2559D-05  1.2675D-07  7.8896D-08  2.8101D-02  4.7545D-08  3.9746D-14  5.2360D-11  8.2007D-03  6.3545D-14
  9.9111D+02  2.1328D-05  1.0776D-07  9.2805D-08  2.6692D-02  1.4605D-08  2.7698D-15  5.2260D-12  5.3566D-03  4.4549D-15
```

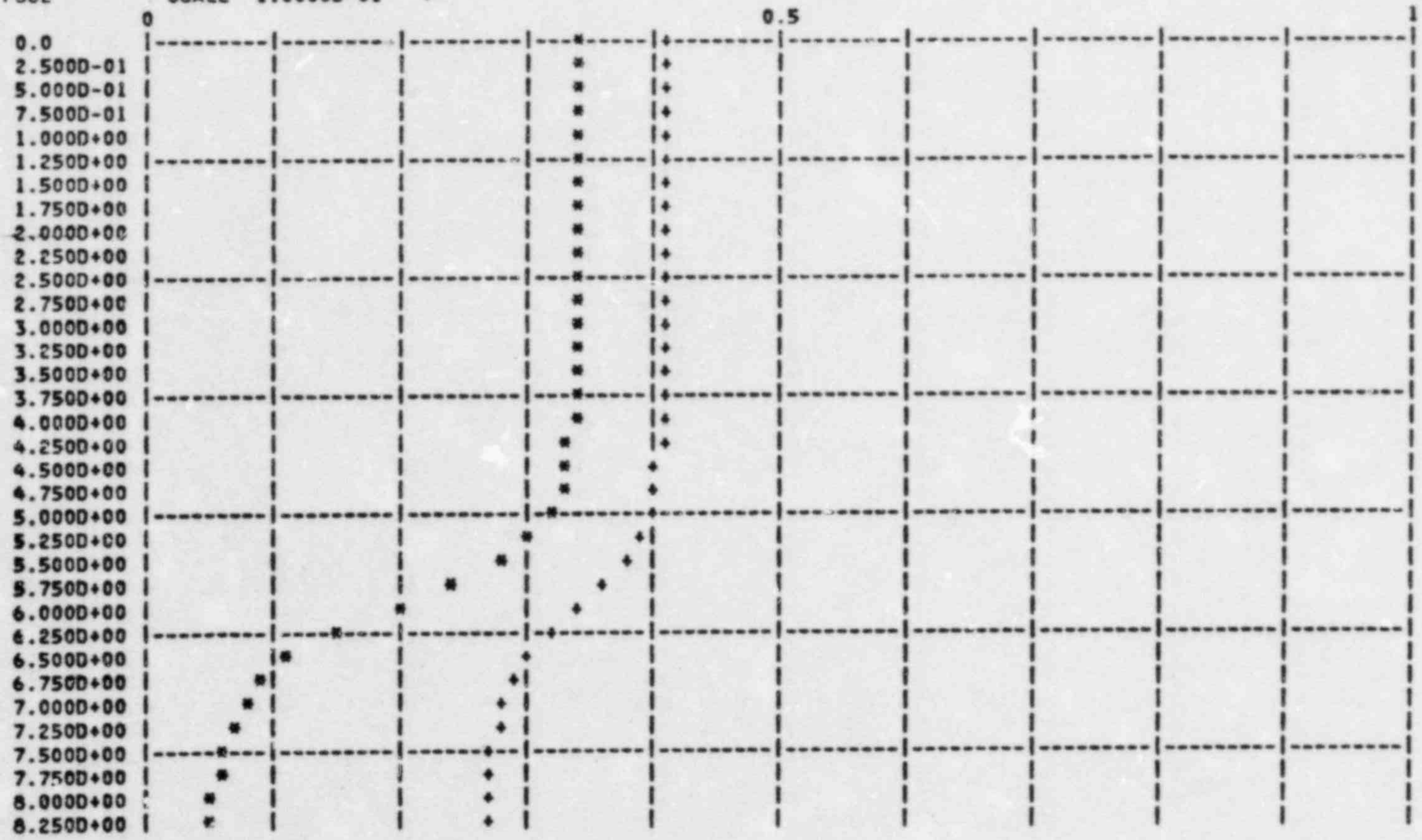
FIG. G-3

```
PRINT STREAM NO.  3
  DOMR        HO2         H2O         HO2-        PO2         PH2         PSO2        PSH2
  2.1789D-03  1.3670D-09  5.5300D+01  3.7817D-11  4.5503D-02  3.7623D-02  4.1000D-02  3.3900D-02
  2.1782D-02  1.2950D-09  5.5300D+01  1.9612D-10  4.5501D-02  3.7622D-02  4.0998D-02  3.3899D-02
  2.1718D-01  1.2154D-09  5.5300D+01  2.2052D-10  4.5467D-02  3.7597D-02  4.0968D-02  3.3876D-02
  2.1181D+00  1.2771D-09  5.5300D+01  2.9636D-10  4.5233D-02  3.7347D-02  4.0757D-02  3.3651D-02
  1.8621D+01  1.1536D-09  5.5302D+01  3.4092D-10  4.4123D-02  3.5201D-02  3.9757D-02  3.1718D-02
  1.2095D+02  7.8779D-10  5.5315D+01  3.3319D-10  3.7611D-02  2.2072D-02  3.3889D-02  1.9888D-02
  5.1569D+02  3.7674D-10  5.5328D+01  3.1336D-10  3.1187D-02  9.1013D-03  2.8101D-02  8.2007D-03
  9.9111D+02  9.8371D-11  5.5332D+01  3.4869D-10  2.9623D-02  5.9449D-03  2.6692D-02  5.3566D-03
```

```
PRINT STREAM NO.  4
  DOMR          TIME          H2T           O2T           H2O2T
  2.1789D-03  1.0000D+01  2.5775D-04  5.0471D-04  4.6287D-08
  2.1782D-02  1.0000D+02  2.5771D-04  5.0441D-04  2.9626D-06
  2.1716D-01  1.0000D+03  2.5750D-04  5.0397D-04  4.3185D-05
  2.1181D+00  1.0000D+04  2.5580D-04  5.0155D-04  2.4357D-04
  1.8621D+01  1.0000D+05  2.4111D-04  4.8931D-04  3.2088D-04
  1.2095D+02  1.0000D+06  1.5119D-04  4.1715D-04  2.7951D-04
  5.1569D+02  1.0000D+07  6.2353D-05  3.4594D-04  2.2110D-04
  9.9111D+02  1.0000D+08  4.0728D-05  3.2859D-04  2.0902D-04
```

```
PRINT STREAM NO.  6
  DOMR         H2O2         H+           OH-          O2           O2-          H            OH           H2           E-
  LH2          LO2          LH2O2        LH+          LO2-         LOH          LHO2         LE-          LH           LHO2-
  2.1789D-03   3.8375D-06   1.7854D-07   5.6037D-08   4.8972D-05   1.2247D-07   3.5029D-13   2.1988D-10   2.5263D-05   5.2933D-13
  1.0402D+01   1.0690D+01   9.5841D+00   8.2517D+00   8.0880D+00   5.3422D+00   6.1358D+00   2.7237D+00   2.5444D+00   4.5777D+00
  2.1782D-02   1.9552D-05   1.7535D-07   5.7040D-08   3.7985D-05   1.1811D-07   4.0058D-13   2.4036D-10   1.8945D-05   5.3146D-13
  1.0277D+01   1.0580D+01   1.0291D+01   8.2439D+00   8.0723D+00   5.3809D+00   6.1123D+00   2.7255D+00   2.6027D+00   5.2925D+00
  2.1718D-01   2.1524D-05   1.7169D-07   5.8253D-08   3.5697D-05   1.1321D-07   3.7314D-13   2.6265D-10   1.3596D-05   5.3819D-13
  1.0133D+01   1.0553D+01   1.0333D+01   8.2347D+00   8.0539D+00   5.4194D+00   6.0847D+00   2.7309D+00   2.5719D+00   5.3434D+00
  2.1181D+00   2.9421D-05   1.7457D-07   5.7279D-08   4.3049D-05   1.1700D-07   2.9243D-13   2.2505D-10   1.4902D-05   4.1053D-13
  1.0173D+01   1.0634D+01   1.0469D+01   8.2420D+00   8.0682D+00   5.3523D+00   6.1062D+00   2.6133D+00   2.4660D+00   5.4718D+00
  1.8621D+01   3.2733D-05   1.6884D-07   5.9216D-08   4.5167D-05   1.0928D-07   2.2511D-13   1.8111D-10   1.5069D-05   3.0823D-13
  1.0178D+01   1.0655D+01   1.0515D+01   8.2275D+00   8.0385D+00   5.2580D+00   6.0621D+00   2.4889D+00   2.5524D+00   5.5326D+00
  1.2095D+02   2.8503D-05   1.5050D-07   6.6437D-08   4.0595D-05   8.3728D-08   1.3456D-13   1.2403D-10   1.1470D-05   1.9156D-13
  1.0060D+01   1.0608D+01   1.0455D+01   8.1775D+00   7.9229D+00   5.0935D+00   5.8964D+00   2.2823D+00   2.1289D+00   5.5227D+00
  5.1569D+02   2.2559D-05   1.2675D-07   7.8896D-08   3.5265D-05   4.7545D-08   3.9746D-14   5.2360D-11   6.2954D-06   6.3545D-14
  9.7990D+00   1.0547D+01   1.0353D+01   8.1030D+00   7.6771D+00   4.7190D+00   5.5760D+00   1.8031D+00   1.5993D+00   5.4960D+00
  9.9111D+02   2.1328D-05   1.0776D-07   9.2805D-08   3.3527D-05   1.4605D-08   2.7698D-15   5.2260D-12   4.1545D-06   4.4549D-15
  9.6185D+00   1.0525D+01   1.0329D+01   8.0325D+00   7.1645D+00   3.7182D+00   4.9929D+00   6.4883D-01   4.4244D-01   5.5424D+00
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2         SCALE  1.0000D-01   *
PSO2         SCALE  1.0000D-01   +
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2           SCALE  2.00000D+01    A
LO2           SCALE  2.00000D+01    B
LH2O2         SCALE  2.00000D+01    C
            0                                                0.5                                                1
 0.0        |---------|---------|---------|---------|--C------|-A-B-----|---------|---------|---------|---------|
 2.5000D-01 |         |         |         |         |   C     | A B     |         |         |         |         |
 5.0000D-01 |         |         |         |         |    C    | A B     |         |         |         |         |
 7.5000D-01 |         |         |         |         |      C  | AB      |         |         |         |         |
 1.0000D+00 |         |         |         |         |       C | AB      |         |         |         |         |
 1.2500D+00 |---------|---------|---------|---------|--------C|-AB------|---------|---------|---------|---------|
 1.5000D+00 |         |         |         |         |         C AB      |         |         |         |         |
 1.7500D+00 |         |         |         |         |         |CAB      |         |         |         |         |
 2.0000D+00 |         |         |         |         |         |C B      |         |         |         |         |
 2.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 2.5000D+00 |---------|---------|---------|---------|---------|ACB------|---------|---------|---------|---------|
 2.7500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 3.0000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 3.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 3.5000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 3.7500D+00 |---------|---------|---------|---------|---------|ACB------|---------|---------|---------|---------|
 4.0000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 4.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 4.5000D+00 |         |         |         |         |         |A C      |         |         |         |         |
 4.7500D+00 |         |         |         |         |         |A C      |         |         |         |         |
 5.0000D+00 |---------|---------|---------|---------|---------|A-C------|---------|---------|---------|---------|
 5.2500D+00 |         |         |         |         |         |A C      |         |         |         |         |
 5.5000D+00 |         |         |         |         |         |A C      |         |         |         |         |
 5.7500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 6.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 6.2500D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 6.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 6.7500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.0000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.2500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.5000D+00 |---------|---------|---------|---------|-------A-|-CB------|---------|---------|---------|---------|
 7.7500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
 8.0000D+00 |         |         |         |         |       A | CB      |         |         |         |         |
 8.2500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 10
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+           SCALE  1.0000D+01   A
LO2-          SCALE  1.0000D+01   B
LOH           SCALE  1.0000D+01   C
LOH-          SCALE  1.0000D+01   D
LHO2          SCALE  1.0000D+01   E
            0                                                0.5                                                1
 0.0        |---------|---------|---------|---------|---------|--C------|E--------|------D--|B-A------|---------|
 2.5000D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
 5.0000D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
 7.5000D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
 1.0000D+00 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
 1.2500D+00 |---------|---------|---------|---------|---------|--C------|E--------|------D--|B-A------|---------|
 1.5000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 1.7500D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 2.0000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 2.2500D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 2.5000D+00 |---------|---------|---------|---------|---------|---C-----|E--------|-------D-|BA-------|---------|
 2.7500D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 3.0000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 3.2500D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 3.5000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 3.7500D+00 |---------|---------|---------|---------|---------|---C-----|E--------|-------D-|BA-------|---------|
 4.0000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
 4.2500D+00 |         |         |         |         |         |  C      |E        |       D |BA       |         |
 4.5000D+00 |         |         |         |         |         |  C      |E        |       D |BA       |         |
 4.7500D+00 |         |         |         |         |         |  C      |E        |       D |BA       |         |
 5.0000D+00 |---------|---------|---------|---------|---------|--C------|E--------|-------D-B-A-------|---------|
 5.2500D+00 |         |         |         |         |         | C       E         |       D B A       |         |
 5.5000D+00 |         |         |         |         |         | C       E         |       D B A       |         |
 5.7500D+00 |         |         |         |         |         |C       E|         |       D B A       |         |
 6.0000D+00 |         |         |         |         |         |C       E|         |       DB| A       |         |
 6.2500D+00 |---------|---------|---------|---------|---------C-------E-|---------|-------DB|-A-------|---------|
 6.5000D+00 |         |         |         |         |         C      E  |         |       BD|A        |         |
 6.7500D+00 |         |         |         |         |       C |      E  |         |      B D|A        |         |
 7.0000D+00 |         |         |         |         |      C  |     E   |         |      B D|A        |         |
 7.2500D+00 |         |         |         |         |    C    |    E    |         |     B  D|A        |         |
 7.5000D+00 |---------|---------|---------|---------|-C-------|--E------|---------|---B----D|A--------|---------|
 7.7500D+00 |         |         |         |        C|         |E        |         | B       D         |         |
 8.0000D+00 |         |         |         |      C  |         E         |         | B       D         |         |
 8.2500D+00 |         |         |         |      C  |         E         |         |B        D         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 11
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-          SCALE  1.0000D+01   A
LH           SCALE  1.0000D+01   B
LHO2-        SCALE  1.0000D+01   C
           0                                                0.5                                                1
 0.0       |---------|---------|----B-A--|-----C---|---------|---------|---------|---------|---------|---------|
 2.500D-01 |         |         |    B A  |       C |         |         |         |         |         |         |
 5.000D-01 |         |         |    B A  |         |C        |         |         |         |         |         |
 7.500D-01 |         |         |    B A  |         |  C      |         |         |         |         |         |
 1.000D+00 |         |         |    B A  |         |     C   |         |         |         |         |         |
 1.250D+00 |---------|---------|-----BA--|---------|-------C-|---------|---------|---------|---------|---------|
 1.500D+00 |         |         |     BA  |         |         C         |         |         |         |         |
 1.750D+00 |         |         |     BA  |         |         | C       |         |         |         |         |
 2.000D+00 |         |         |     BA  |         |         |  C      |         |         |         |         |
 2.250D+00 |         |         |     BA  |         |         |  C      |         |         |         |         |
 2.500D+00 |---------|---------|-----BA--|---------|---------|--C------|---------|---------|---------|---------|
 2.750D+00 |         |         |     BA  |         |         |  C      |         |         |         |         |
 3.000D+00 |         |         |     BA  |         |         |  C      |         |         |         |         |
 3.250D+00 |         |         |     BA  |         |         |   C     |         |         |         |         |
 3.500D+00 |         |         |    B A  |         |         |   C     |         |         |         |         |
 3.750D+00 |---------|---------|----B-A--|---------|---------|---C-----|---------|---------|---------|---------|
 4.000D+00 |         |         |    BA   |         |         |    C    |         |         |         |         |
 4.250D+00 |         |         |   B A   |         |         |    C    |         |         |         |         |
 4.500D+00 |         |         |   B A   |         |         |    C    |         |         |         |         |
 4.750D+00 |         |         |   BA    |         |         |    C    |         |         |         |         |
 5.000D+00 |---------|---------|---BA----|---------|---------|----C----|---------|---------|---------|---------|
 5.250D+00 |         |         |  BA     |         |         |    C    |         |         |         |         |
 5.500D+00 |         |         | B A     |         |         |    C    |         |         |         |         |
 5.750D+00 |         |         | BA      |         |         |    C    |         |         |         |         |
 6.000D+00 |         |         |B A      |         |         |    C    |         |         |         |         |
 6.250D+00 |---------|---------B-A-------|---------|---------|----C----|---------|---------|---------|---------|
 6.500D+00 |         |        B|A        |         |         |    C    |         |         |         |         |
 6.750D+00 |         |       B A         |         |         |    C    |         |         |         |         |
 7.000D+00 |         |     B A |         |         |         |    C    |         |         |         |         |
 7.250D+00 |         |   B A   |         |         |         |    C    |         |         |         |         |
 7.500D+00 |---------B-A-------|---------|---------|---------|----C----|---------|---------|---------|---------|
 7.750D+00 |     B A |         |         |         |         |    C    |         |         |         |         |
 8.000D+00 |   B A   |         |         |         |         |    C    |         |         |         |         |
 8.250D+00 |   B A   |         |         |         |         |    C    |         |         |         |         |
```

APPENDIX H

CORE VOLUMETRIC FLOW RATE

SENSITIVITY ANALYSIS

This appendix documents the results of sensitivity calculations carried out for various core volumetric flow rates. Increasing the core volumetric flow rate increases the rate at which concentrations of H_2, O_2, and H_2O_2 tend to equilibriate between the core and torus.

Variations in core volumetric flow rate are obtained by varying the rate constant k, where:

$$k = \frac{1}{T_M} = \frac{\dot{v}_{core}}{V_{core}} \qquad \text{(H-1)}$$

Assuming: $V_{core} = 2.658 \times 10^5$ liters = 70,219 gal and: $\dot{v}_{core} = 1000$ gpm = 16.667 gal/sec., then: $k = 2.37352 \times 10^{-4}\ \text{sec}^{-1}$. Identical equilibriation rates core input for H_2, O_2, and H_2O_2. The table below summarizes the various case studies performed.

Simulation	Figure	Assumptions
CASE I	Fig. H-1	$\dot{v}_{core} = 10^3$ gpm ($k \cong 2.37 \times 10^{-4}$)
CASE II	Fig. H-2	$\dot{v}_{core} = 10^2$ gpm ($k \cong 2.37 \times 10^{-5}$)
CASE III	Fig. H-3	$\dot{v}_{core} = 10^5$ gpm ($k \cong 2.37 \times 10^{-2}$)

- All other assumptions are as noted in Figure XVII of Section 4.2 in Vol. I.

```
PRINT STREAM NO.  2
  DOMR        H2O2        H+          OH-         PSO2        O2-         H           OH          PSH2        E-
  2.17890-03  3.47310-06  1.78600-07  5.60200-08  4.10000-02  1.22540-07  3.49030-13  2.19520-10  3.39000-02  5.29300-13
  2.17820-02  1.14020-05  1.77370-07  5.64000-08  4.09890-02  1.20860-07  3.68930-13  2.27170-10  3.38950-02  5.21390-13
  2.17180-01  2.26550-05  1.79430-07  5.57400-08  4.08810-02  1.23460-07  3.37380-13  2.12740-10  3.38290-02  4.35880-13
  2.11810+00  4.09060-05  1.81750-07  5.50040-08  4.05130-02  1.26350-07  2.87830-13  1.82600-10  3.33150-02  3.34500-13
  1.86280+01  3.87020-05  1.72500-07  5.79550-08  3.84890-02  1.14150-07  2.37840-13  1.59700-10  2.92290-02  2.81860-13
  1.20960+02  2.65600-05  1.49550-07  6.68720-08  3.09130-02  8.23630-08  1.38280-13  1.29960-10  1.38890-02  2.02460-13
  5.15680+02  2.25180-05  1.26740-07  7.89040-08  2.80490-02  4.75260-08  3.97520-14  5.24320-11  8.09470-03  6.36250-14
  9.90910+02  2.13270-05  1.07760-07  9.28050-08  2.66900-02  1.46050-08  2.76970-15  5.22660-12  5.35380-03  4.45520-15
```

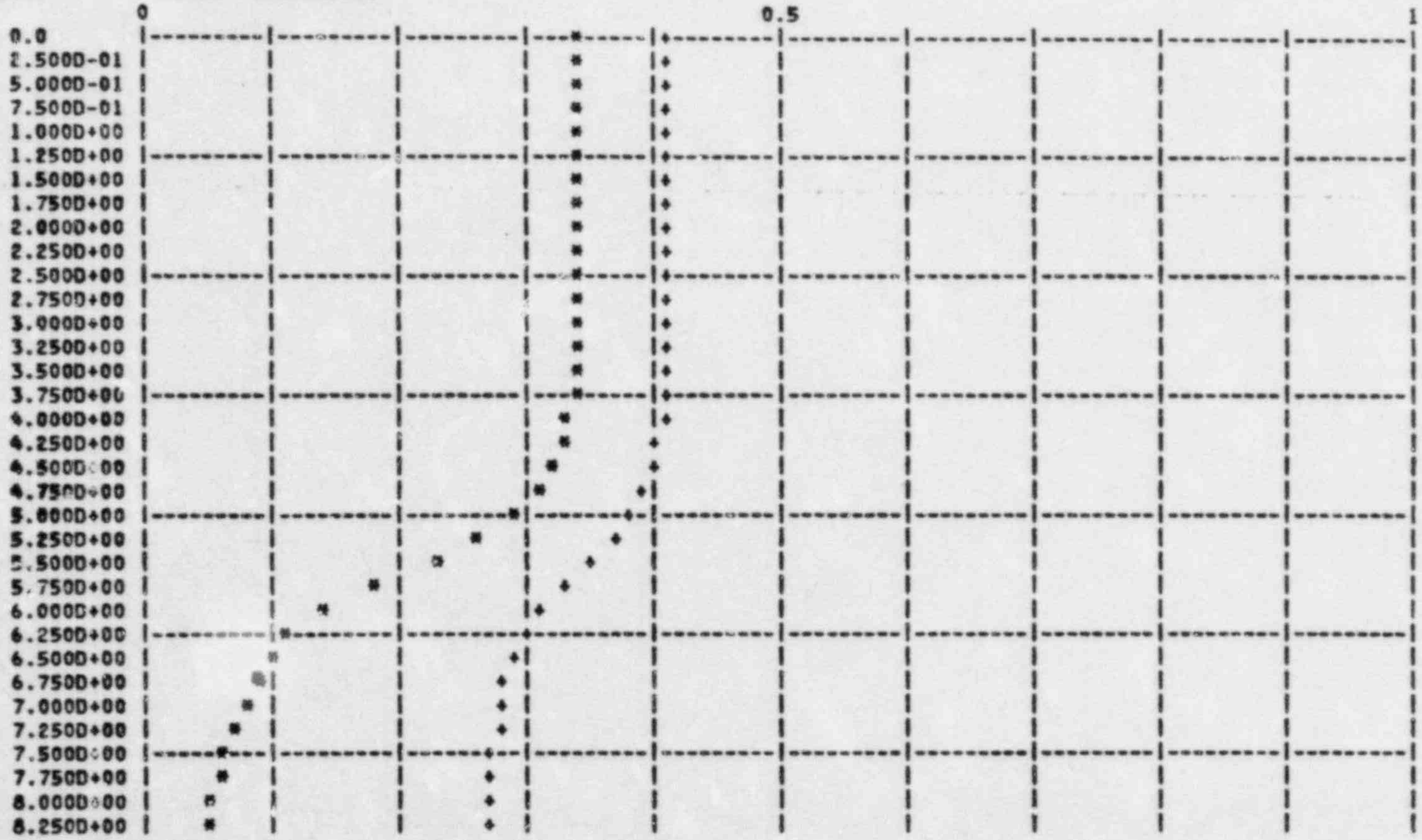
FIG. H-1

```
PRINT STREAM NO.  3
  DOMR        HO2         H2O         HO2-        PO2         PH2         PSO2        PSH2
  2.1789D-03  1.3683D-09  5.5300D+01  3.4216D-11  4.5503D-02  3.7623D-02  4.1000D-02  3.3900D-02
  2.1782D-02  1.3402D-09  5.5300D+01  1.1308D-10  4.5491D-02  3.7617D-02  4.0989D-02  3.3895D-02
  2.1716D-01  1.3851D-09  5.5300D+01  2.2203D-10  4.5371D-02  3.7544D-02  4.0881D-02  3.3829D-02
  2.1181D+00  1.4359D-09  5.5300D+01  3.9557D-10  4.4962D-02  3.6974D-02  4.0513D-02  3.3315D-02
  1.8628D+01  1.2311D-09  5.5305D+01  3.9443D-10  4.2716D-02  3.2439D-02  3.8489D-02  2.9229D-02
  1.2096D+02  7.7009D-10  5.5322D+01  3.1249D-10  3.4308D-02  1.5414D-02  3.0912D-02  1.3889D-02
  5.1568D+02  3.7655D-10  5.5329D+01  3.1281D-10  3.1129D-02  8.9837D-03  2.8049D-02  8.0947D-03
  9.9091D+02  9.8373D-11  5.5332D+01  3.4868D-10  2.9622D-02  5.9418D-03  2.6690D-02  5.3538D-03
```

```
PRINT STREAM NO.  4
  DOMR         TIME         H2T          O2T          H2O2T
  2.1789D-03   1.0000D+01   2.5775D-04   5.0468D-04   4.2981D-07
  2.1782D-02   1.0000D+02   2.5770D-04   5.0443D-04   1.8025D-05
  2.1718D-01   1.0000D+03   2.5720D-04   5.0316D-04   1.7066D-04
  2.1181D+00   1.0000D+04   2.5330D-04   4.9870D-04   4.0030D-04
  1.8628D+01   1.0000D+05   2.2223D-04   4.7380D-04   3.7941D-04
  1.2096D+02   1.0000D+06   1.0560D-04   3.8055D-04   2.6033D-04
  5.1568D+02   1.0000D+07   6.1547D-05   3.4529D-04   2.2069D-04
  9.9091D+02   1.0000D+08   4.0707D-05   3.2857D-04   2.0902D-04
```

```
PRINT STREAM NO.  6
  DOMR        H2O2        H+          OH-         O2          O2-         H           OH          H2          E-
  LH2         LO2         LH2O2       LH+         LO2-        LOH         LHO2        LE-         LH          LHO2-
  2.1789D-03  3.4731D-06  1.7860D-07  5.6020D-08  4.9224D-05  1.2254D-07  3.4903D-13  2.1952D-10  2.5366D-05  5.2930D-13
  1.0404D+01  1.0692D+01  9.5407D+00  8.2519D+00  8.0883D+00  5.3415D+00  6.1362D+00  2.7237D+00  2.5429D+00  4.5342D+00
  2.1782D-02  1.1402D-05  1.7737D-07  5.6400D-08  4.4555D-05  1.2086D-07  3.6893D-13  2.2717D-10  2.2840D-05  5.2139D-13
  1.0359D+01  1.0649D+01  1.0057D+01  8.2489D+00  8.0823D+00  5.3563D+00  6.1272D+00  2.7172D+00  2.5669D+00  5.0534D+00
  2.1718D-01  2.2655D-05  1.7943D-07  5.5740D-08  4.6813D-05  1.2346D-07  3.3738D-13  2.1274D-10  2.2972D-05  4.3588D-13
  1.0361D+01  1.0670D+01  1.0355D+01  8.2539D+00  8.0915D+00  5.3279D+00  6.1415D+00  2.6394D+00  2.5281D+00  5.3464D+00
  2.1181D+00  4.0906D-05  1.8175D-07  5.5004D-08  4.9603D-05  1.2635D-07  2.8783D-13  1.8260D-10  2.3348D-05  3.3450D-13
  1.0368D+01  1.0696D+01  1.0612D+01  8.2595D+00  8.1016D+00  5.2615D+00  6.1571D+00  2.5244D+00  2.4591D+00  5.5972D+00
  1.8628D+01  3.8702D-05  1.7250D-07  5.7955D-08  4.7422D-05  1.1415D-07  2.3784D-13  1.5970D-10  2.0818D-05  2.8186D-13
  1.0318D+01  1.0676D+01  1.0588D+01  8.2368D+00  8.0575D+00  5.2033D+00  6.0903D+00  2.4500D+00  2.3763D+00  5.5960D+00
  1.2096D+02  2.6560D-05  1.4955D-07  6.6872D-08  3.8679D-05  8.2363D-08  1.3828D-13  1.2996D-10  1.0473D-05  2.0246D-13
  1.0020D+01  1.0587D+01  1.0424D+01  8.1748D+00  7.9157D+00  5.1138D+00  5.8865D+00  2.3063D+00  2.1408D+00  5.4948D+00
  5.1568D+02  2.2518D-05  1.2674D-07  7.8904D-08  3.5229D-05  4.7526D-08  3.9752D-14  5.2432D-11  6.2743D-06  6.3625D-14
  9.7976D+00  1.0547D+01  1.0353D+01  8.1029D+00  7.6769D+00  4.7196D+00  5.5758D+00  1.8036D+00  1.5994D+00  5.4953D+00
  9.9091D+02  2.1327D-05  1.0776D-07  9.2805D-08  3.3526D-05  1.4605D-08  2.7697D-15  5.2266D-12  4.1534D-06  4.4552D-15
  9.6184D+00  1.0525D+01  1.0329D+01  8.0325D+00  7.1645D+00  3.7182D+00  4.9929D+00  6.4886D-01  4.4243D-01  5.5424D+00
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2          SCALE  1.00000D-01   *
PSO2          SCALE  1.00000D-01   +
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG       (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2           SCALE  2.0000D+01    A
LO2           SCALE  2.0000D+01    B
LH2O2         SCALE  2.0000D+01    C
           0                                                0.5                                                1
0.0        |---------|---------|---------|---------|--C------|-A-B-----|---------|---------|---------|---------|
2.5000D-01 |         |         |         |         |   C     | A B     |         |         |         |         |
5.0000D-01 |         |         |         |         |    C    | A B     |         |         |         |         |
7.5000D-01 |         |         |         |         |      C  | AB      |         |         |         |         |
1.0000D+00 |         |         |         |         |       C | AB      |         |         |         |         |
1.2500D+00 |---------|---------|---------|---------|--------C|-AB------|---------|---------|---------|---------|
1.5000D+00 |         |         |         |         |        C| AB      |         |         |         |         |
1.7500D+00 |         |         |         |         |         C AB      |         |         |         |         |
2.0000D+00 |         |         |         |         |         C AB      |         |         |         |         |
2.2500D+00 |         |         |         |         |         |CAB      |         |         |         |         |
2.5000D+00 |---------|---------|---------|---------|---------|CAB------|---------|---------|---------|---------|
2.7500D+00 |         |         |         |         |         |CAB      |         |         |         |         |
3.0000D+00 |         |         |         |         |         | CB      |         |         |         |         |
3.2500D+00 |         |         |         |         |         | CB      |         |         |         |         |
3.5000D+00 |         |         |         |         |         | AC      |         |         |         |         |
3.7500D+00 |---------|---------|---------|---------|---------|-AC------|---------|---------|---------|---------|
4.0000D+00 |         |         |         |         |         | AC      |         |         |         |         |
4.2500D+00 |         |         |         |         |         | AC      |         |         |         |         |
4.5000D+00 |         |         |         |         |         | AC      |         |         |         |         |
4.7500D+00 |         |         |         |         |         | AC      |         |         |         |         |
5.0000D+00 |---------|---------|---------|---------|---------|-AC------|---------|---------|---------|---------|
5.2500D+00 |         |         |         |         |         |A C      |         |         |         |         |
5.5000D+00 |         |         |         |         |         |A C      |         |         |         |         |
5.7500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
6.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
6.2500D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
6.5000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
6.7500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.0000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.2500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.5000D+00 |---------|---------|---------|---------|-------A-|-CB------|---------|---------|---------|---------|
7.7500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
8.0000D+00 |         |         |         |         |       A | CB      |         |         |         |         |
8.2500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 10
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+          SCALE  1.00000D+01   A
LO2-         SCALE  1.00000D+01   B
LOH          SCALE  1.00000D+01   C
LOH-         SCALE  1.00000D+01   D
LHO2         SCALE  1.00000D+01   E
          0                                                0.5                                                1
0.0       |---------|---------|---------|---------|---------|--C------|E--------|------D--|B-A------|---------|
2.500D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
5.000D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
7.500D-01 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
1.000D+00 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
1.250D+00 |---------|---------|---------|---------|---------|--C------|E--------|------D--|B-A------|---------|
1.500D+00 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
1.750D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
2.000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
2.250D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
2.500D+00 |---------|---------|---------|---------|---------|---C-----|E--------|-------D-|BA-------|---------|
2.750D+00 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
3.000D+00 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
3.250D+00 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
3.500D+00 |         |         |         |         |         |  C      | E       |      D  |B A      |         |
3.750D+00 |---------|---------|---------|---------|---------|--C------|-E-------|------D--|B-A------|---------|
4.000D+00 |         |         |         |         |         |  C      | E       |      D  |B A      |         |
4.250D+00 |         |         |         |         |         |  C      |E        |      D  |B A      |         |
4.500D+00 |         |         |         |         |         | C       |E        |      D  |B A      |         |
4.750D+00 |         |         |         |         |         | C       |E        |       D |BA       |         |
5.000D+00 |---------|---------|---------|---------|---------|-C-------|E--------|-------D-|BA-------|---------|
5.250D+00 |         |         |         |         |         | C       E         |       D B A       |         |
5.500D+00 |         |         |         |         |         |C        E         |       D B A       |         |
5.750D+00 |         |         |         |         |         |C       E|         |       D B A       |         |
6.000D+00 |         |         |         |         |         |C       E|         |       DB| A       |         |
6.250D+00 |---------|---------|---------|---------|---------|C------E-|---------|-------DB|-A-------|---------|
6.500D+00 |         |         |         |         |         C      E  |         |       BD|A        |         |
6.750D+00 |         |         |         |         |        C|      E  |         |      B D|A        |         |
7.000D+00 |         |         |         |         |      C  |     E   |         |      B D|A        |         |
7.250D+00 |         |         |         |         |    C    |    E    |         |     B  D|A        |         |
7.500D+00 |---------|---------|---------|---------|-C-------|--E------|---------|---B----D|A--------|---------|
7.750D+00 |         |         |         |        C|         |E        |         | B       D         |         |
8.000D+00 |         |         |         |      C  |         E         |         | B       D         |         |
8.250D+00 |         |         |         |      C  |         E         |         |B        D         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 11
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-          SCALE  1.0000D+01   A
LK           SCALE  1.0000D+01   B
LHO2-        SCALE  1.0000D+01   C
            0                                                0.5                                                1
 0.0        |---------|---------|----B-A--|-----C---|---------|---------|---------|---------|---------|---------|
 2.5000D-01 |         |         |    B A  |       C |         |         |         |         |         |         |
 5.0000D-01 |         |         |    B A  |         |C        |         |         |         |         |         |
 7.5000D-01 |         |         |    B A  |         |  C      |         |         |         |         |         |
 1.0000D+00 |         |         |    B A  |         |    C    |         |         |         |         |         |
 1.2500D+00 |---------|---------|-----BA--|---------|------C--|---------|---------|---------|---------|---------|
 1.5000D+00 |         |         |     BA  |         |        C|         |         |         |         |         |
 1.7500D+00 |         |         |     BA  |         |         C         |         |         |         |         |
 2.0000D+00 |         |         |     BA  |         |         |C        |         |         |         |         |
 2.2500D+00 |         |         |     BA  |         |         |C        |         |         |         |         |
 2.5000D+00 |---------|---------|-----BA--|---------|---------|-C-------|---------|---------|---------|---------|
 2.7500D+00 |         |         |    B A  |         |         | C       |         |         |         |         |
 3.0000D+00 |         |         |    BA   |         |         |  C      |         |         |         |         |
 3.2500D+00 |         |         |    BA   |         |         |   C     |         |         |         |         |
 3.5000D+00 |         |         |    BA   |         |         |    C    |         |         |         |         |
 3.7500D+00 |---------|---------|----B----|---------|---------|-----C---|---------|---------|---------|---------|
 4.0000D+00 |         |         |    B    |         |         |     C   |         |         |         |         |
 4.2500D+00 |         |         |   BA    |         |         |     C   |         |         |         |         |
 4.5000D+00 |         |         |   BA    |         |         |     C   |         |         |         |         |
 4.7500D+00 |         |         |   BA    |         |         |     C   |         |         |         |         |
 5.0000D+00 |---------|---------|---BA----|---------|---------|-----C---|---------|---------|---------|---------|
 5.2500D+00 |         |         |  BA     |         |         |     C   |         |         |         |         |
 5.5000D+00 |         |         |  BA     |         |         |     C   |         |         |         |         |
 5.7500D+00 |         |         | BA      |         |         |    C    |         |         |         |         |
 6.0000D+00 |         |         |B A      |         |         |    C    |         |         |         |         |
 6.2500D+00 |---------|---------B-A-------|---------|---------|----C----|---------|---------|---------|---------|
 6.5000D+00 |         |        B|A        |         |         |    C    |         |         |         |         |
 6.7500D+00 |         |       B A         |         |         |    C    |         |         |         |         |
 7.0000D+00 |         |     B A |         |         |         |    C    |         |         |         |         |
 7.2500D+00 |         |   B A   |         |         |         |    C    |         |         |         |         |
 7.5000D+00 |---------B-A-------|---------|---------|---------|----C----|---------|---------|---------|---------|
 7.7500D+00 |     B A |         |         |         |         |    C    |         |         |         |         |
 8.0000D+00 |   B A   |         |         |         |         |    C    |         |         |         |         |
 8.2500D+00 |   B A   |         |         |         |         |    C    |         |         |         |         |
```

```
PRINT STREAM NO.  2
  DOMR        H2O2        H+          OH-         PSO2        O2-         H           OH          PSH2        E-
  2.1789D-03  3.8771D-06  1.7854D-07  5.6039D-08  4.1000D-02  1.2246D-07  3.5042D-13  2.1992D-10  3.3900D-02  5.2933D-13
  2.1782D-02  2.1077D-05  1.7501D-07  5.7149D-08  4.1000D-02  1.1765D-07  4.0625D-13  2.4264D-10  3.3900D-02  5.3251D-13
  2.1718D-01  2.0880D-05  1.6803D-07  5.9521D-08  4.0996D-02  1.0829D-07  3.6491D-13  2.8901D-10  3.3897D-02  5.7609D-13
  2.1182D+00  2.1621D-05  1.6731D-07  5.9776D-08  4.0962D-02  1.0730D-07  3.3701D-13  2.7434D-10  3.3866D-02  5.3191D-13
  1.8618D+01  2.6841D-05  1.6465D-07  6.0725D-08  4.0721D-02  1.0364D-07  2.2162D-13  2.0755D-10  3.3565D-02  3.4797D-13
  1.2094D+02  2.7918D-05  1.4995D-07  6.6665D-08  3.9298D-02  8.2961D-08  1.2145D-13  1.2743D-10  3.0751D-02  1.8731D-13
  5.1558D+02  2.4674D-05  1.2729D-07  7.8551D-08  3.1450D-02  4.8395D-08  3.8768D-14  4.9051D-11  1.4950D-02  5.9453D-14
  9.9134D+02  2.1367D-05  1.0776D-07  9.2803D-08  2.6716D-02  1.4608D-08  2.7715D-15  5.2171D-12  5.4063D-03  4.4507D-15
```

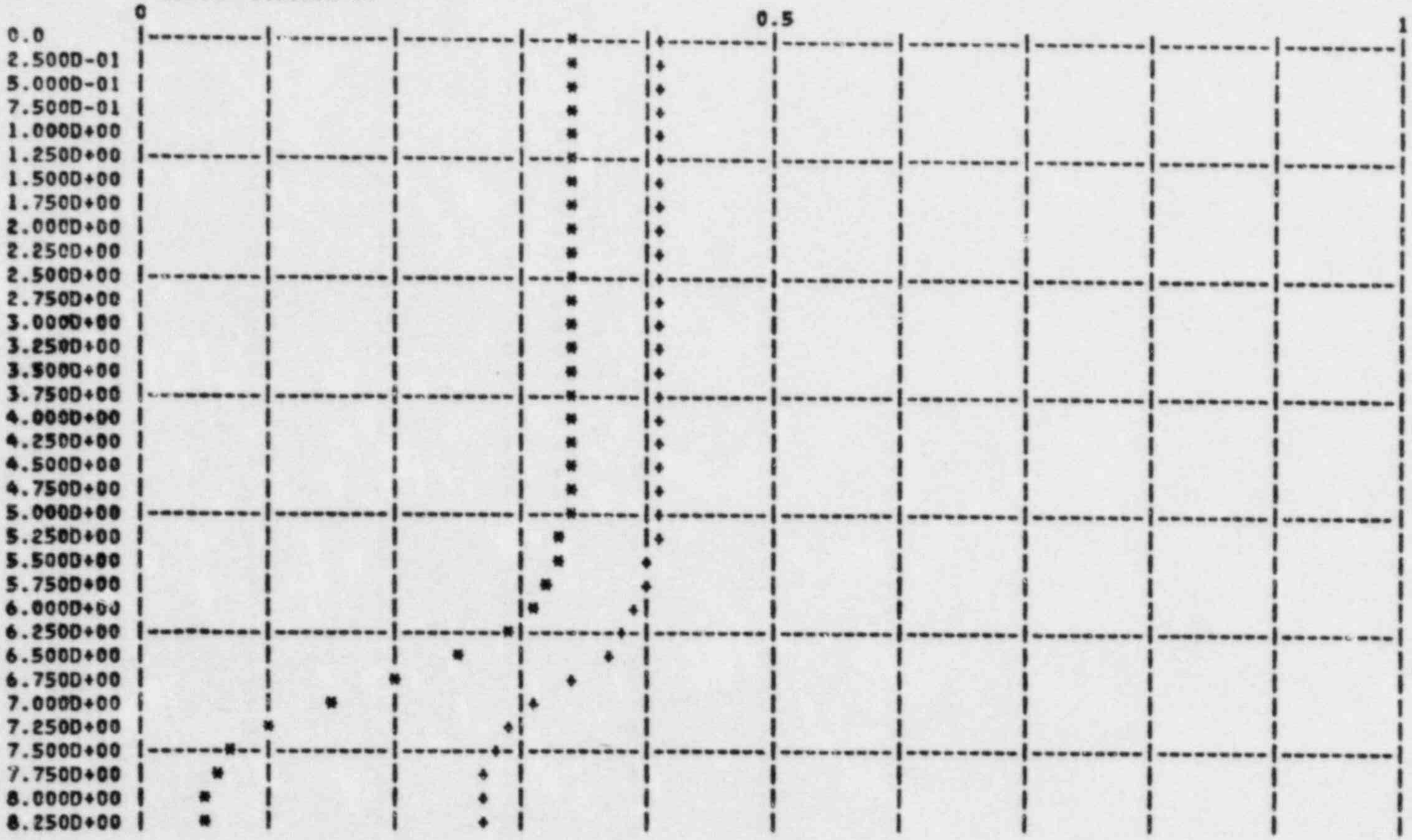
FIG. H-2

```
PRINT STREAM NO.  3
  DOMR        HO2         H2O         HO2-        PO2         PH2         PSO2        PSH2
  2.1789D-03  1.3669D-09  5.5300D+01  3.8208D-11  4.5503D-02  3.7623D-02  4.1000D-02  3.3900D-02
  2.1782D-02  1.2874D-09  5.5300D+01  2.1182D-10  4.5503D-02  3.7623D-02  4.1000D-02  3.3900D-02
  2.1718D-01  1.1378D-09  5.5300D+01  2.1860D-10  4.5499D-02  3.7620D-02  4.0996D-02  3.3897D-02
  2.1182D+00  1.1225D-09  5.5300D+01  2.2734D-10  4.5460D-02  3.7585D-02  4.0962D-02  3.3866D-02
  1.8618D+01  1.0670D-09  5.5300D+01  2.8673D-10  4.5194D-02  3.7251D-02  4.0721D-02  3.3565D-02
  1.2094D+02  7.7779D-10  5.5303D+01  3.2756D-10  4.3614D-02  3.4126D-02  3.9298D-02  3.0751D-02
  5.1558D+02  3.8509D-10  5.5321D+01  3.4128D-10  3.4904D-02  1.6592D-02  3.1450D-02  1.4950D-02
  9.9134D+02  9.8394D-11  5.5332D+01  3.4933D-10  2.9650D-02  6.0001D-03  2.6716D-02  5.4063D-03
```

```
PRINT STREAM NO.  4
  DOMR         TIME         H2T          O2T          H2O2T
  2.17890-03  1.00000D+01  2.57760-04  5.04730-04  4.66370-09
  2.17820-02  1.00000D+02  2.57750-04  5.04730-04  3.14850-07
  2.17180-01  1.00000D+03  2.57730-04  5.04680-04  4.91100-06
  2.11820+00  1.00000D+04  2.57490-04  5.04260-04  4.46100-05
  1.86180+01  1.00000D+05  2.55210-04  5.01300-04  2.28020-04
  1.20940+02  1.00000D+06  2.33810-04  4.83780-04  2.73810-04
  5.15580+02  1.00000D+07  1.13670-04  3.87170-04  2.41930-04
  9.91340+02  1.00000D+08  4.11060-05  3.28890-04  2.09420-04
```

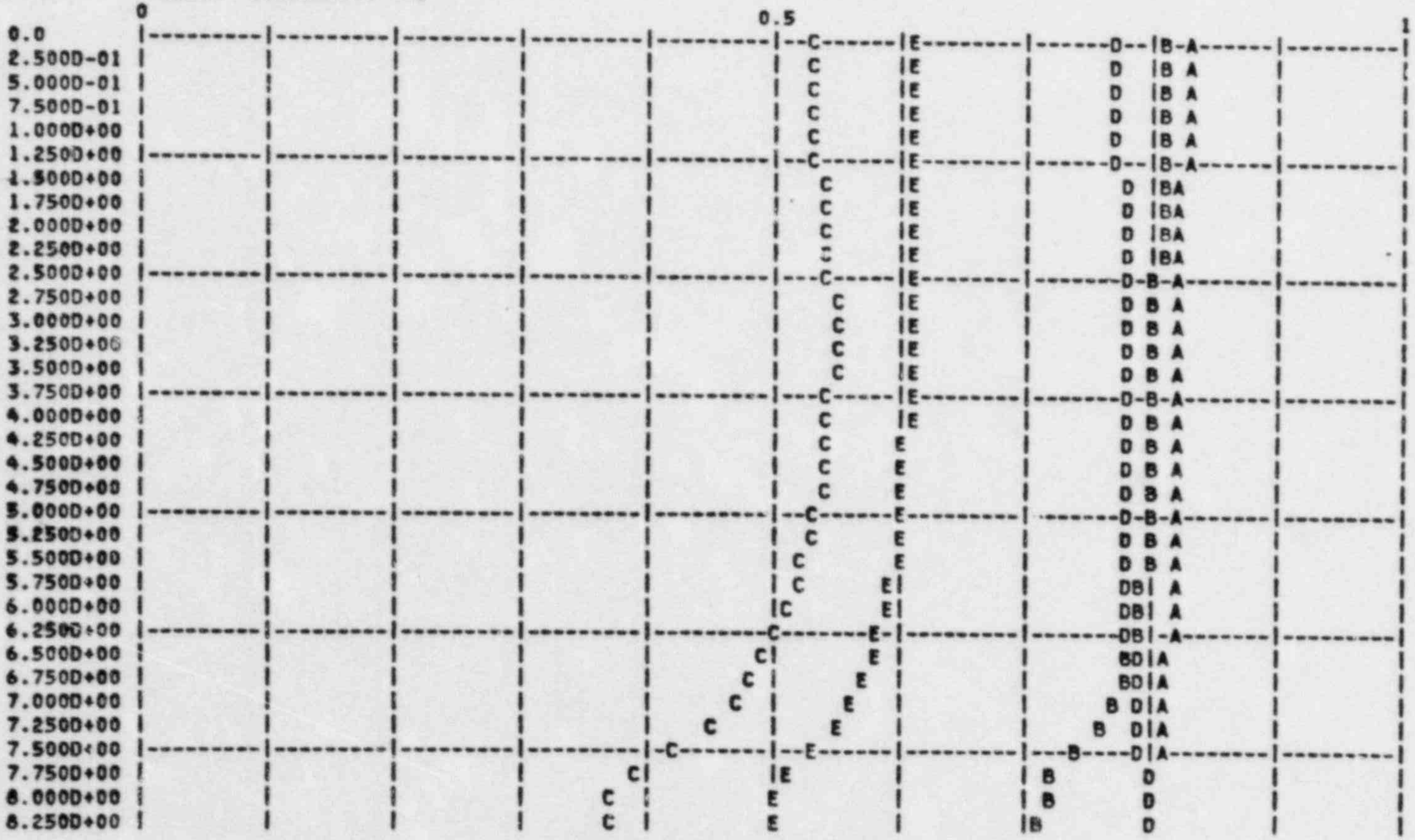
```
PRINT STREAM NO.  6
  DOMR        H2O2        H+          OH-         O2          O2-         H           OH          H2          E-
  LH2         LO2         LH2O2       LH+         LO2-        LOH         LHO2        LE-         LH          LHO2-
  2.1789D-03  3.8771D-06  1.7854D-07  5.6039D-08  4.8944D-05  1.2246D-07  3.5042D-13  2.1992D-10  2.5252D-05  5.2933D-13
  1.0402D+01  1.0690D+01  9.5885D+00  8.2517D+00  8.0880D+00  5.3423D+00  6.1357D+00  2.7237D+00  2.5446D+00  4.5822D+00
  2.1782D-02  2.1077D-05  1.7501D-07  5.7149D-08  3.6840D-05  1.1765D-07  4.0625D-13  2.4264D-10  1.8231D-05  5.3251D-13
  1.0261D+01  1.0566D+01  1.0324D+01  8.2431D+00  8.0706D+00  5.3850D+00  6.1097D+00  2.7263D+00  2.6088D+00  5.3260D+00
  2.1718D-01  2.0880D-05  1.6803D-07  5.9521D-08  3.2867D-05  1.0829D-07  3.6491D-13  2.8901D-10  9.8699D-06  5.7609D-13
  9.9943D+00  1.0516D+01  1.0320D+01  8.2254D+00  8.0346D+00  5.4609D+00  6.0561D+00  2.7605D+00  2.5622D+00  5.3397D+00
  2.1182D+00  2.1621D-05  1.6731D-07  5.9776D-08  3.3915D-05  1.0730D-07  3.3701D-13  2.7434D-10  9.9355D-06  5.3191D-13
  9.9972D+00  1.0530D+01  1.0335D+01  8.2235D+00  8.0306D+00  5.4383D+00  6.0502D+00  2.7258D+00  2.5276D+00  5.3567D+00
  1.8618D+01  2.6841D-05  1.6465D-07  6.0725D-08  4.1459D-05  1.0364D-07  2.2162D-13  2.0755D-10  1.0615D-05  3.4797D-13
  1.0026D+01  1.0618D+01  1.0429D+01  8.2166D+00  8.0155D+00  5.3171D+00  6.0282D+00  2.5415D+00  2.3456D+00  5.4575D+00
  1.2094D+02  2.7918D-05  1.4995D-07  6.6665D-08  4.2369D-05  8.2961D-08  1.2145D-13  1.2743D-10  9.8427D-06  1.8731D-13
  9.9931D+00  1.0627D+01  1.0446D+01  8.1760D+00  7.9189D+00  5.1053D+00  5.8909D+00  2.2726D+00  2.0844D+00  5.5153D+00
  5.1558D+02  2.4674D-05  1.2729D-07  7.8551D-08  3.7321D-05  4.8395D-08  3.8768D-14  4.9051D-11  7.2181D-06  5.9453D-14
  9.8584D+00  1.0572D+01  1.0392D+01  8.1048D+00  7.6846D+03  4.6906D+00  5.5856D+00  1.7742D+00  1.5885D+00  5.5331D+00
  9.9134D+02  2.1367D-05  1.0776D-07  9.2803D-08  3.3548D-05  1.4608D-08  2.7715D-15  5.2171D-12  4.1732D-06  4.4507D-15
  9.6205D+00  1.0526D+01  1.0330D+01  8.0325D+00  7.1646D+00  3.7174D+00  4.9930D+00  6.4843D-01  4.4272D-01  5.5432D+00
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2          SCALE  1.00000D-01   *
FSO2          SCALE  1.00000D-01   +
```

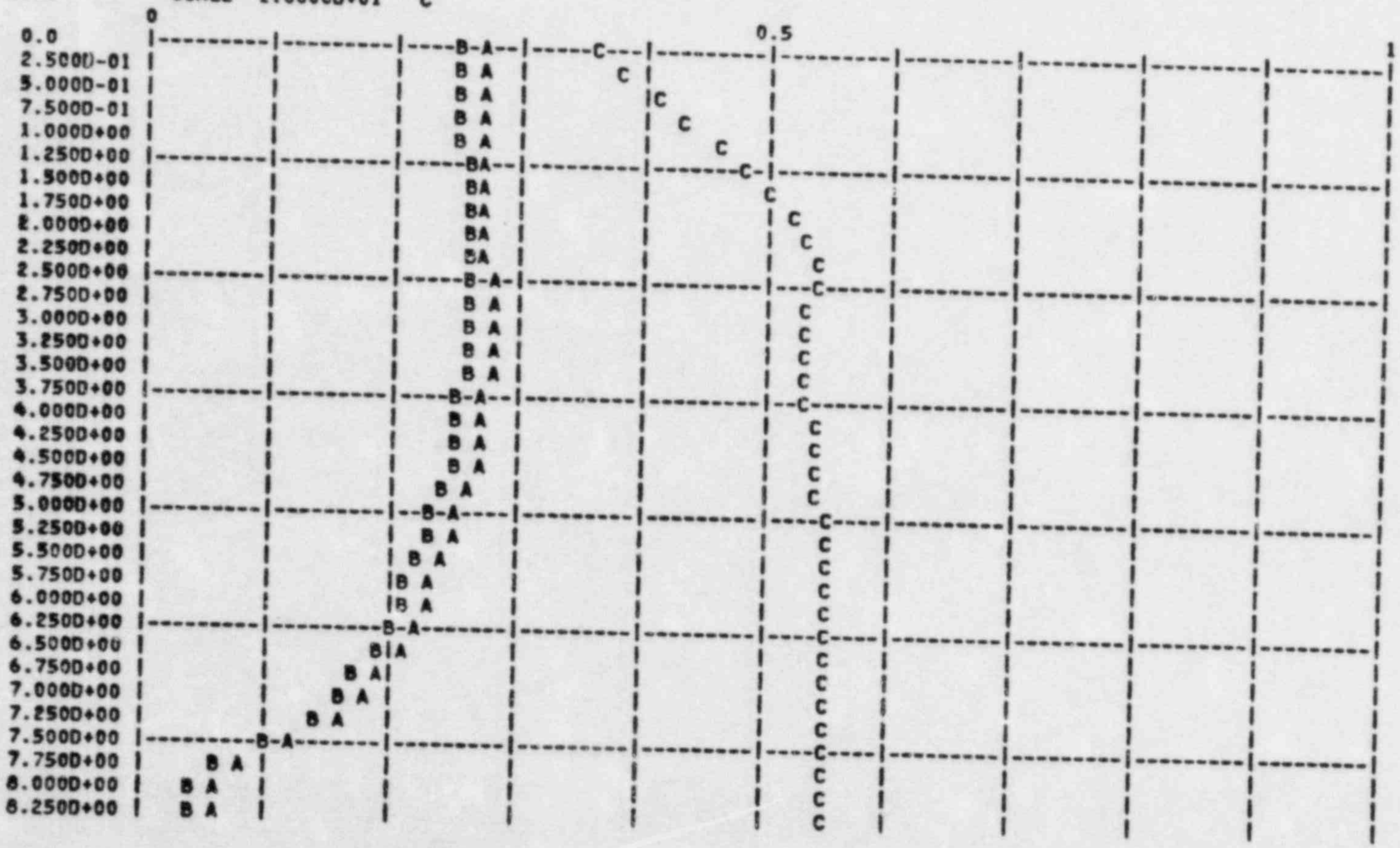


```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2           SCALE  2.0000D+01   A
LO2           SCALE  2.0000D+01   B
LH2O2         SCALE  2.0000D+01   C
           0                                                0.5                                                1
0.0        |---------|---------|---------|---------|--C------|-A-B-----|---------|---------|---------|---------|
2.5000D-01 |         |         |         |         |   C     | A B     |         |         |         |         |
5.0000D-01 |         |         |         |         |     C   | A B     |         |         |         |         |
7.5000D-01 |         |         |         |         |      C  | AB      |         |         |         |         |
1.0000D+00 |         |         |         |         |       C | AB      |         |         |         |         |
1.2500D+00 |---------|---------|---------|---------|--------C|-AB------|---------|---------|---------|---------|
1.5000D+00 |         |         |         |         |         C AB      |         |         |         |         |
1.7500D+00 |         |         |         |         |         |CAB      |         |         |         |         |
2.0000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
2.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
2.5000D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
2.7500D+00 |         |         |         |         |         A CB      |         |         |         |         |
3.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
3.2500D+00 |         |         |         |         |         A CB      |         |         |         |         |
3.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
3.7500D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
4.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
4.2500D+00 |         |         |         |         |         A CB      |         |         |         |         |
4.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
4.7500D+00 |         |         |         |         |         A CB      |         |         |         |         |
5.0000D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
5.2500D+00 |         |         |         |         |         A CB      |         |         |         |         |
5.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
5.7500D+00 |         |         |         |         |         A CB      |         |         |         |         |
6.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
6.2500D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
6.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
6.7500D+00 |         |         |         |         |         A CB      |         |         |         |         |
7.0000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.2500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
7.5000D+00 |---------|---------|---------|---------|--------A|-CB------|---------|---------|---------|---------|
7.7500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
8.0000D+00 |         |         |         |         |       A | CB      |         |         |         |         |
8.2500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 10
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+           SCALE  1.0000D+01   A
LO2-          SCALE  1.0000D+01   B
LOH           SCALE  1.0000D+01   C
LOH-          SCALE  1.0000D+01   D
LHO2          SCALE  1.0000D+01   E
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM 11
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-          SCALE  1.0000D+01   A
LH           SCALE  1.0000D+01   B
LHO2-        SCALE  1.0000D+01   C
```



```
PRINT STREAM NO.  2
  DCMR         H2O2         H+           OH-          PSO2         O2-          H            OH           PSH2         E-
  2.1789D-03   3.8811D-06   1.7854D-07   5.6039D-08   4.1000D-02   1.2246D-07   3.5044D-13   2.1992D-10   3.3900D-02   5.2933D-13
  2.1782D-02   2.1242D-05   1.7497D-07   5.7161D-08   4.1000D-02   1.1760D-07   4.0686D-13   2.4288D-10   3.3900D-02   5.3262D-13
  2.1718D-01   2.0822D-05   1.6760D-07   5.9675D-08   4.1000D-02   1.0770D-07   3.6196D-13   2.9229D-10   3.3900D-02   5.7943D-13
  2.1185D+00   2.0797D-05   1.6621D-07   6.0171D-08   4.0996D-02   1.0582D-07   3.4551D-13   2.8243D-10   3.3896D-02   5.5349D-13
  1.8622D+01   2.1400D-05   1.6059D-07   6.2269D-08   4.0961D-02   9.8087D-08   2.6939D-13   2.3557D-10   3.3864D-02   4.3170D-13
  1.2097D+02   2.5968D-05   1.4894D-07   6.7117D-08   4.0708D-02   8.1519D-08   1.2284D-13   1.3384D-10   3.3533D-02   1.9699D-13
  5.1574D+02   2.6376D-05   1.2759D-07   7.8336D-08   3.9074D-02   4.8894D-08   3.4518D-14   4.7188D-11   3.0285D-02   5.4677D-14
  9.9160D+02   2.4171D-05   1.0787D-07   9.2690D-08   3.0311D-02   1.4785D-08   2.7438D-15   4.6587D-12   1.2657D-02   4.0958D-15
```

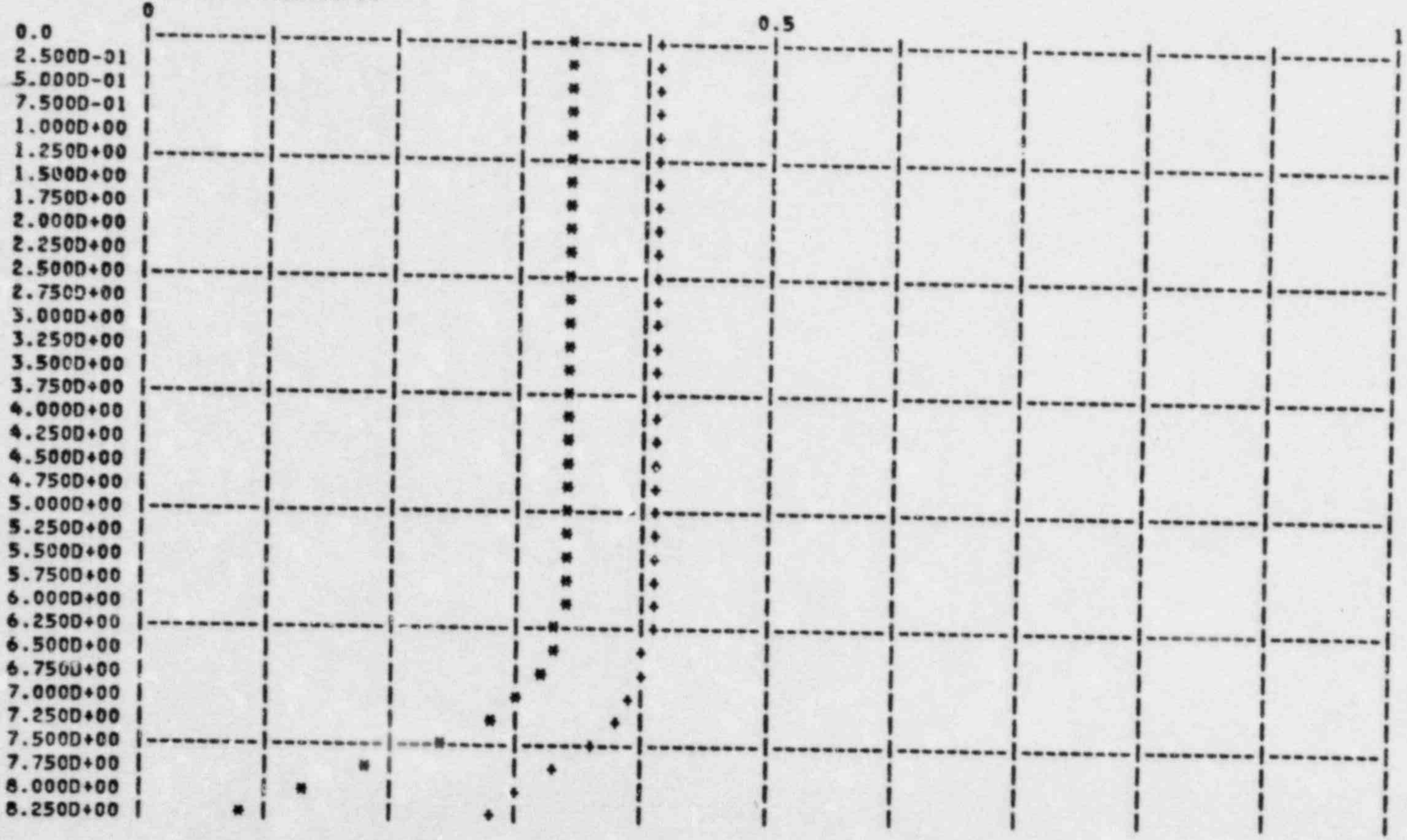
FIG. H-3

```
PRINT STREAM NO.  3
  DOMR         HO2          H2O          HO2-         PO2          PH2          PSO2         PSH2
  2.1789D-03   1.3669D-09   5.5300D+01   3.8248D-11   4.5503D-02   3.7623D-02   4.1000D-02   3.3900D-02
  2.1782D-02   1.2866D-09   5.5300D+01   2.1352D-10   4.5503D-02   3.7623D-02   4.1000D-02   3.3900D-02
  2.1718D-01   1.1287D-09   5.5300D+01   2.1857D-10   4.5502D-02   3.7623D-02   4.1000D-02   3.3900D-02
  2.1185D+00   1.0998D-09   5.5300D+01   2.2013D-10   4.5498D-02   3.7619D-02   4.0996D-02   3.3896D-02
  1.8622D+01   9.8491D-10   5.5300D+01   2.3445D-10   4.5459D-02   3.7583D-02   4.0961D-02   3.3864D-02
  1.2097D+02   7.5912D-10   5.5300D+01   3.0677D-10   4.5179D-02   3.7215D-02   4.0708D-02   3.3533D-02
  5.1574D+02   3.8999D-10   5.5304D+01   3.6392D-10   4.3365D-02   3.3611D-02   3.9074D-02   3.0285D-02
  9.9160D+02   9.9683D-11   5.5323D+01   3.9473D-10   3.3640D-02   1.4047D-02   3.0311D-02   1.2657D-02
```

```
PRINT STREAM NO.  4
  DOMR         TIME         H2T          O2T          H2O2T
  2.1789D-03   1.0000D+01   2.5776D-04   5.0473D-04   4.6672D-10
  2.1782D-02   1.0000D+02   2.5776D-04   5.0473D-04   3.1681D-08
  2.1718D-01   1.0000D+03   2.5775D-04   5.0473D-04   4.9767D-07
  2.1185D+00   1.0000D+04   2.5773D-04   5.0468D-04   4.8755D-06
  1.8622D+01   1.0000D+05   2.5748D-04   5.0425D-04   4.4292D-05
  1.2097D+02   1.0000D+06   2.5496D-04   5.0114D-04   2.2188D-04
  5.1574D+02   1.0000D+07   2.3027D-04   4.8102D-04   2.5874D-04
  9.9160D+02   1.0000D+08   9.6236D-05   3.7315D-04   2.3704D-04
```

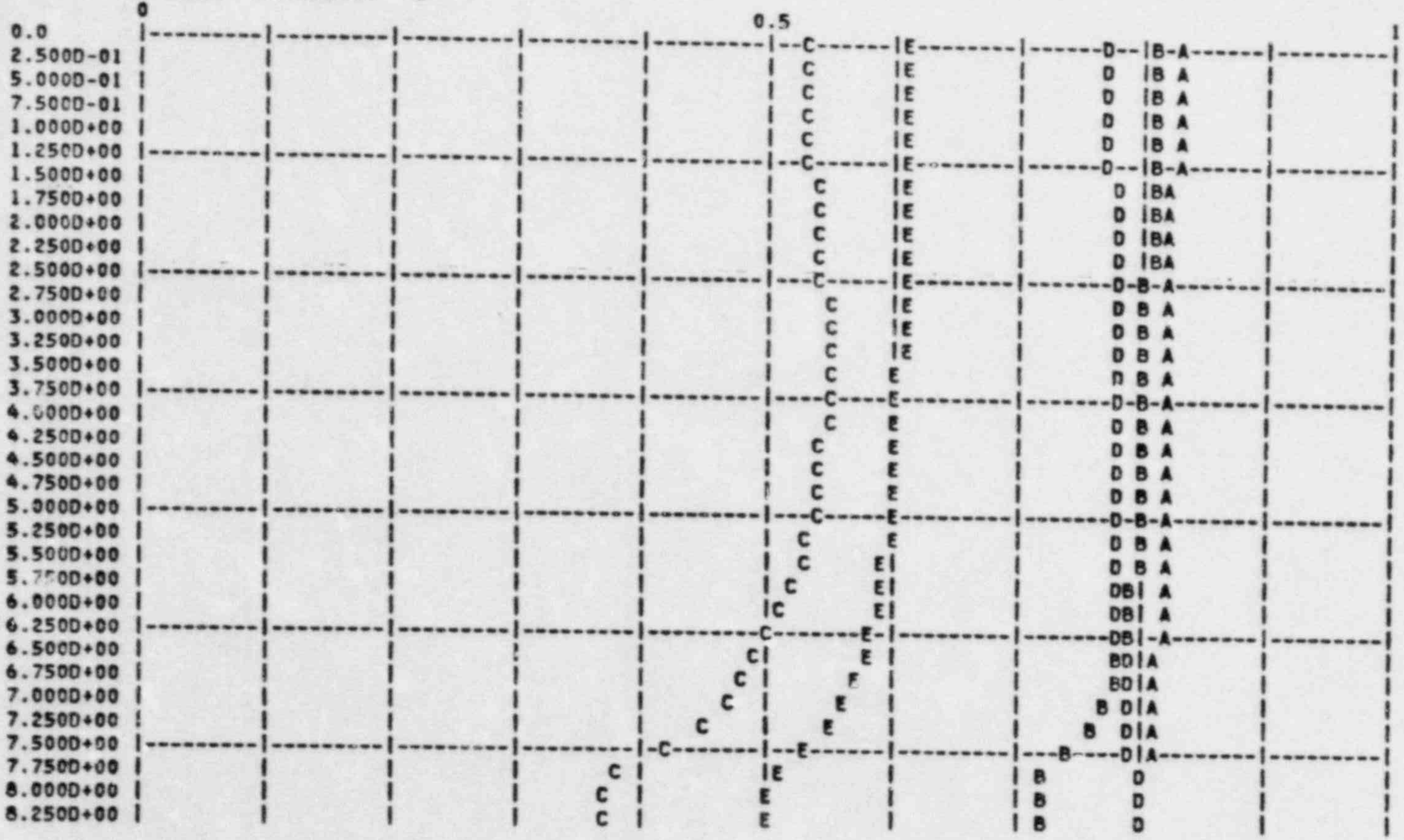
```
PRINT STREAM NO.  6
  DOMR        H2O2        H+          OH-         O2          O2-         H           OH          H2          E-
  LH2         LO2         LH2O2       LH+         LO2-        LOH         LHO2        LE-         LH          LHO2-
  2.1789D-03  3.8811D-06  1.7854D-07  5.6039D-08  4.8942D-05  1.2246D-07  3.5044D-13  2.1992D-10  2.5250D-05  5.2933D-13
  1.0402D+01  1.0690D+01  9.5890D+00  8.2517D+00  8.0890D+00  5.3423D+00  6.1357D+00  2.7237D+00  2.5446D+00  4.5826D+00
  2.1782D-02  2.1242D-05  1.7497D-07  5.7161D-08  3.6717D-05  1.1760D-07  4.0686D-13  2.4288D-10  1.8154D-05  5.3262D-13
  1.0259D+01  1.0565D+01  1.0327D+01  8.2430D+00  8.0704D+00  5.3854D+00  6.1094D+00  2.7264D+00  2.6094D+00  5.3294D+00
  2.1716D-01  2.0822D-05  1.6760D-07  5.9675D-08  3.2574D-05  1.0770D-07  3.6196D-13  2.9229D-10  9.4288D-06  5.7943D-13
  9.9745D+00  1.0513D+01  1.0319D+01  8.2243D+00  8.0322D+00  5.4658D+00  6.0526D+00  2.7630D+00  2.5587D+00  5.3396D+00
  2.1185D+00  2.0797D-05  1.6621D-07  6.0171D-08  3.2571D-05  1.0582D-07  3.4551D-13  2.8243D-10  9.3117D-06  5.5349D-13
  9.9690D+00  1.0513D+01  1.0318D+01  8.2207D+00  8.0246D+00  5.4509D+00  6.0413D+00  2.7431D+00  2.5385D+00  5.3427D+00
  1.8622D+01  2.1400D-05  1.6059D-07  6.2269D-08  3.3533D-05  9.8087D-08  2.6939D-13  2.3557D-10  8.9702D-06  4.3170D-13
  9.9528D+00  1.0525D+01  1.0330D+01  8.2057D+00  7.9916D+00  5.3721D+00  5.9934D+00  2.6352D+00  2.4304D+00  5.3700D+00
  1.2097D+02  2.5968D-05  1.4894D-07  6.7117D-08  4.0667D-05  8.1519D-08  1.2284D-13  1.3384D-10  8.7661D-06  1.9699D-13
  9.9428D+00  1.0609D+01  1.0414D+01  8.1730D+00  7.9113D+00  5.1266D+00  5.8803D+00  2.2945D+00  2.0893D+00  5.4868D+00
  3.1574D+02  2.6376D-05  1.2759D-07  7.8336D-08  4.0910D-05  4.8894D-08  3.4518D-14  4.7188D-11  7.1205D-06  5.4677D-14
  9.8525D+00  1.0612D+01  1.0421D+01  8.1058D+00  7.6893D+00  4.6738D+00  5.5911D+00  1.7378D+00  1.5380D+00  5.5610D+00
  9.9160D+02  2.4171D-05  1.0787D-07  9.2690D-08  3.5816D-05  1.4785D-08  2.7438D-15  4.6587D-12  5.2843D-06  4.0958D-15
  9.7230D+00  1.0554D+01  1.0383D+01  8.0329D+00  7.1698D+00  3.6683D+00  4.9986D+00  6.1234D-01  4.3835D-01  5.5963D+00
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2          SCALE  1.00000D-01   *
PSO2          SCALE  1.00000D-01   +
```

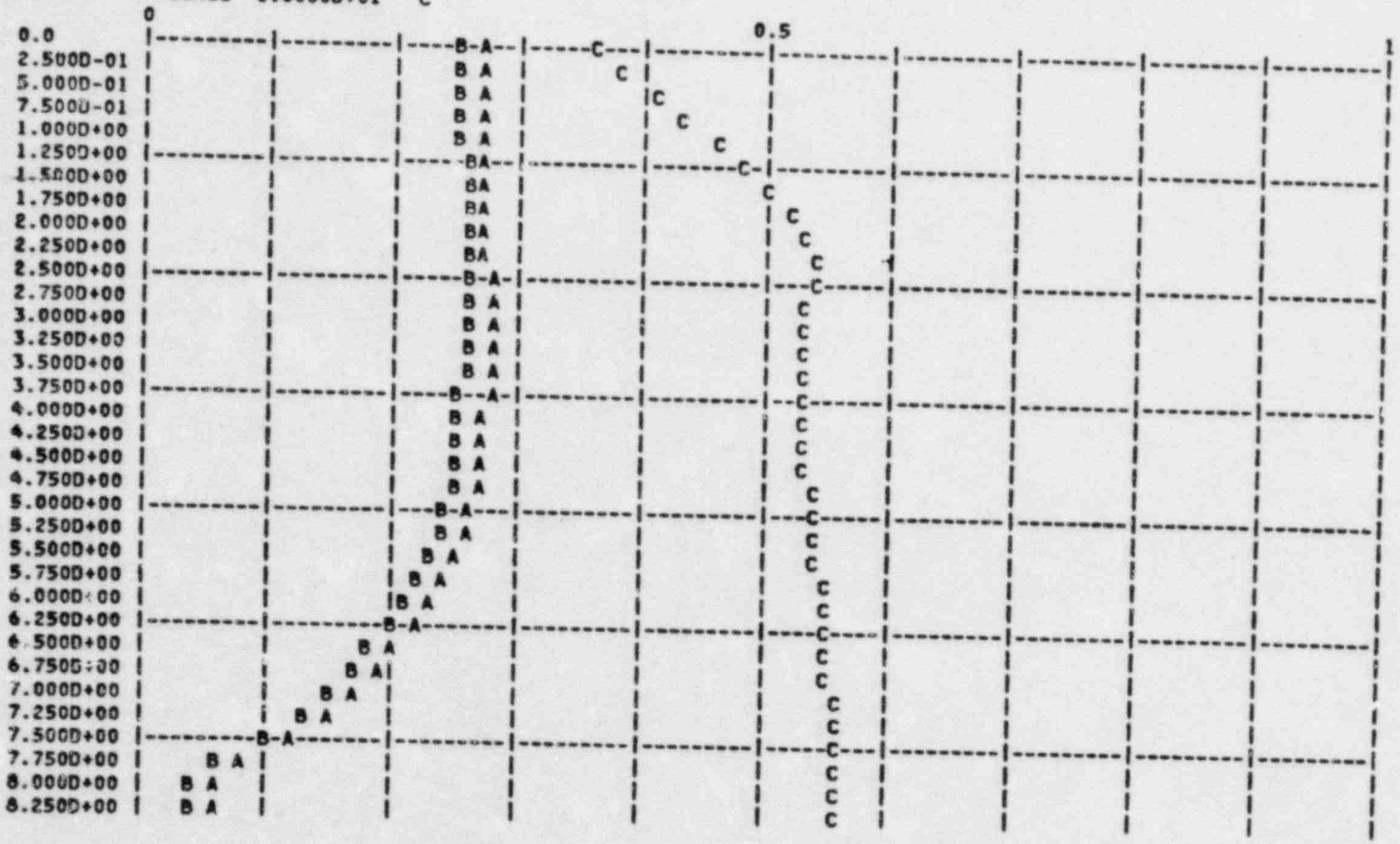


```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2          SCALE  2.0000D+01   A
LO2          SCALE  2.0000D+01   B
LH2O2        SCALE  2.00000D+01  C
            0                                                0.5                                                1
 0.0        |---------|---------|---------|---------|--C------|-A-B-----|---------|---------|---------|---------|
 2.5000D-01 |         |         |         |         |   C     | A B     |         |         |         |         |
 5.0000D-01 |         |         |         |         |     C   | A B     |         |         |         |         |
 7.5000D-01 |         |         |         |         |      C  | AB      |         |         |         |         |
 1.0000D+00 |         |         |         |         |       C | AB      |         |         |         |         |
 1.2500D+00 |---------|---------|---------|---------|--------C|-AB------|---------|---------|---------|---------|
 1.5000D+00 |         |         |         |         |         C AB      |         |         |         |         |
 1.7500D+00 |         |         |         |         |         |CAB      |         |         |         |         |
 2.0000D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 2.2500D+00 |         |         |         |         |         |ACB      |         |         |         |         |
 2.5000D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 2.7500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 3.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 3.2500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 3.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 3.7500D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 4.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 4.2500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 4.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 4.7500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 5.0000D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 5.2500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 5.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 5.7500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 6.0000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 6.2500D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 6.5000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 6.7500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.0000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.2500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.5000D+00 |---------|---------|---------|---------|--------A|-CB------|---------|---------|---------|---------|
 7.7500D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 8.0000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 8.2500D+00 |         |         |         |         |       A | CB      |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 10
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+          SCALE  1.0000D+01   A
LO2-         SCALE  1.0000D+01   B
LOH          SCALE  1.0000D+01   C
LOH-         SCALE  1.0000D+01   D
LHO2         SCALE  1.0000D+01   Z
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM II
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-         SCALE  1.0000D+01   A
LH          SCALE  1.0000D+01   B
LHO2-       SCALE  1.0000D+01   C
```



APPENDIX I

EXTENT OF $Zr-H_2O$ REACTION

SENSITIVITY ANALYSIS

This Appendix documents the results of the sensitivity analysis to the extent of the metal-water reaction. Two specific cases were evaluated. The first cast is for $f_{Zr-H_2O} = 0.0$ with $\varepsilon_{H_2O} = 110$ lbs. H_2O. The results of this case shown in Figure I-1 indicate that the rate of recombination is quite slow due to the low initial H_2 overpressure. As f_{Zr-H_2O} is increased to 0.00612 (with $\varepsilon_{H_2O} = 110$ lbs. H_2O) there is a slight increase in the net rate of recombination. This case is documented in Figure I-2.

```
PRINT STREAM NO.  2
  DOMR         H2O2         H+           OH-          PSO2         O2-          H            OH           PSH2         E-
  2.1789D-03   3.2158D-06   1.6724D-07   5.9825D-08   3.6900D-02   1.0738D-07   3.0757D-13   2.9709D-10   1.6600D-03   5.8445D-13
  2.1782D-02   1.6064D-05   1.6850D-07   5.9362D-08   3.6899D-02   1.0897D-07   3.3650D-13   2.8792D-10   1.6597D-03   5.6512D-13
  2.1716D-01   1.9872D-05   1.6888D-07   5.9222D-08   3.6879D-02   1.0945D-07   3.3215D-13   2.8269D-10   1.6551D-03   5.4328D-13
  2.1181D+00   2.6699D-05   1.7165D-07   5.8257D-08   3.6770D-02   1.1312D-07   2.6339D-13   2.4412D-10   1.6207D-03   4.2160D-13
  1.8619D+01   2.9393D-05   1.6609D-07   6.0198D-08   3.6656D-02   1.0558D-07   1.9799D-13   1.9830D-10   1.4673D-03   3.1599D-13
  1.2092D+02   2.9213D-05   1.5034D-07   6.6488D-08   3.6517D-02   8.3511D-08   1.0841D-13   1.2505D-10   1.2040D-03   1.7480D-13
  5.1563D+02   2.9058D-05   1.2808D-07   7.8030D-08   3.6381D-02   4.9647D-08   3.0422D-14   4.4355D-11   9.4538D-04   4.9139D-14
  9.9130D+02   2.8905D-05   1.0799D-07   9.2537D-08   3.6244D-02   1.4982D-08   2.0300D-15   4.0548D-12   6.8664D-04   3.2835D-15
```

FIG. I-1

$f_{Zr-H_2O} = 0.00$

```
PRINT STREAM NO.  3
  DOMR         HO2          H2O          HO2-         PO2          PH2          PSO2         PSH2
  2.1789D-03   1.1227D-09   5.5300D+01   3.3845D-11   4.0953D-02   1.8423D-03   3.6900D-02   1.6600D-03
  2.1782D-02   1.1480D-09   5.5300D+01   1.6773D-10   4.0951D-02   1.8420D-03   3.6899D-02   1.6597D-03
  2.1718D-01   1.1558D-09   5.5300D+01   2.0700D-10   4.0929D-02   1.8369D-03   3.6879D-02   1.6551D-03
  2.1181D+00   1.2141D-09   5.5300D+01   2.7355D-10   4.0809D-02   1.7987D-03   3.6770D-02   1.6207D-03
  1.8619D+01   1.0964D-09   5.5300D+01   3.1125D-10   4.0682D-02   1.6284D-03   3.6656D-02   1.4673D-03
  1.2092D+02   7.8496D-10   5.5300D+01   3.4186D-10   4.0528D-02   1.3362D-03   3.6517D-02   1.2040D-03
  5.1563D+02   3.9750D-10   5.5301D+01   3.9937D-10   4.0376D-02   1.0492D-03   3.6381D-02   9.4538D-04
  9.9130D+02   1.0113D-10   5.5301D+01   4.7146D-10   4.0224D-02   7.6205D-04   3.6244D-02   6.8664D-04
```

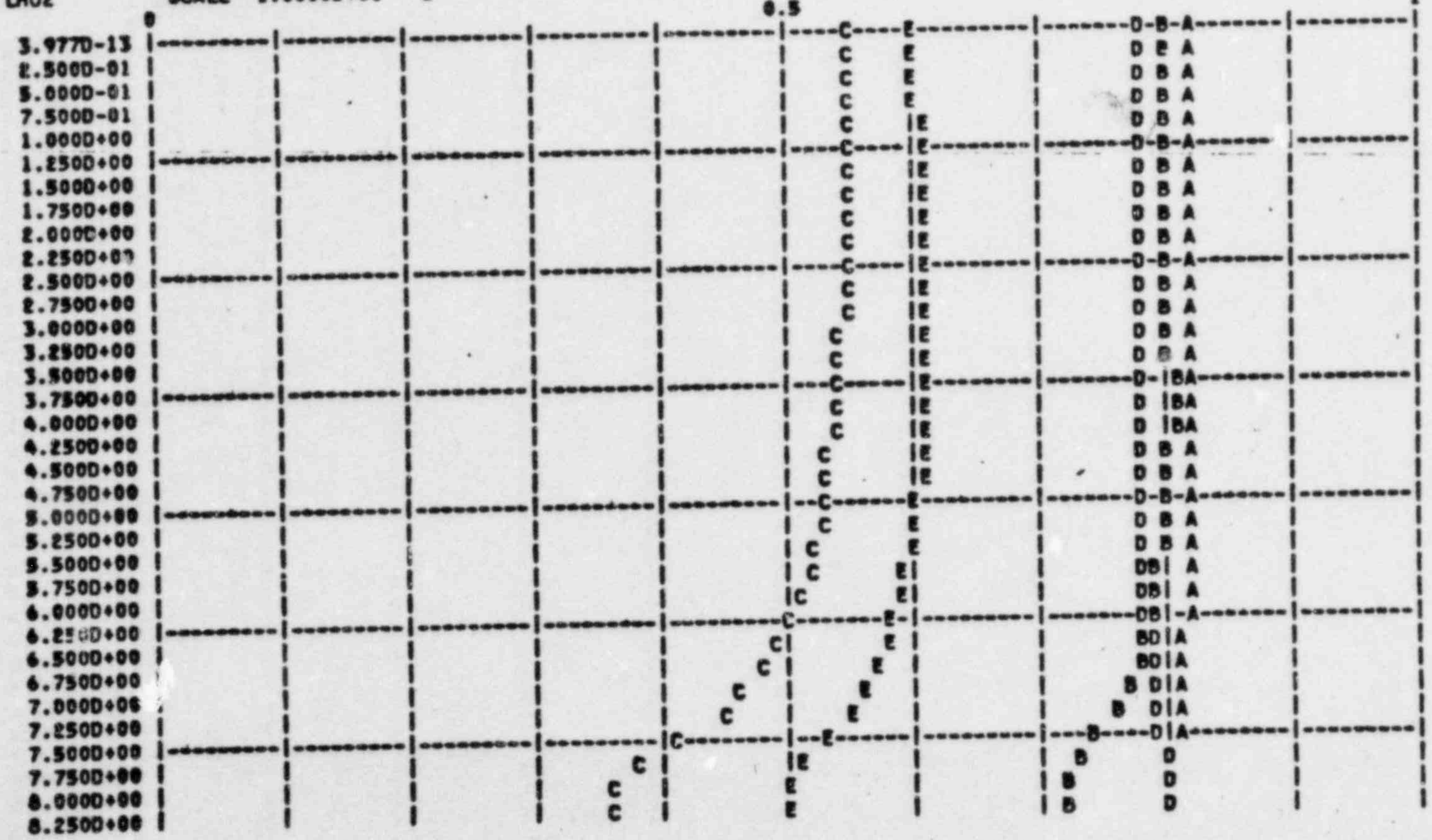
```
PRINT STREAM NO.  4
  DOMR          TIME          H2T           O2T           H2O2T
  2.1789D-03   1.00000D+01   1.2643D-04   4.5474D-04   3.8923D-08
  2.1782D-02   1.00000D+02   1.2641D-04   4.5471D-04   2.4360D-06
  2.1717D-01   1.00000D+03   1.2605D-04   4.5447D-04   3.8847D-05
  2.1181D+00   1.00000D+04   1.2343D-04   4.5314D-04   2.2189D-04
  1.8619D+01   1.00000D+05   1.1175D-04   4.5174D-04   2.8808D-04
  1.2092D+02   1.00000D+06   9.1699D-05   4.5003D-04   2.8631D-04
  5.1563D+02   1.00000D+07   7.2001D-05   4.4835D-04   2.8478D-04
  9.9130D+02   1.00000D+08   5.2295D-05   4.4666D-04   2.8328D-04
```

```
PRINT STREAM NO.  6
  DOMR         H2O2         H+           OH-          O2           O2-          H            OH           H2           E-
  LH2          LO2          LH2O2        LH+          LO2-         LOH          LHO2         LE-          LH           LHO2-
  2.1789D-03   3.2158D-06   1.6724D-07   5.9825D-08   4.4520D-05   1.0738D-07   3.0757D-13   2.9709D-10   1.2515D-05   5.8445D-13
  1.0097D+01   1.0649D+01   9.5073D+00   8.2233D+00   8.0309D+00   5.4729D+00   6.0503D+00   2.7667D+00   2.4879D+00   4.5295D+00
  2.1782D-02   1.6064D-05   1.6850D-07   5.9362D-08   3.7305D-05   1.0897D-07   3.3650D-13   2.8792D-10   1.0884D-05   5.6512D-13
  1.0037D+01   1.0572D+01   1.0206D+01   8.2266D+00   8.0373D+00   5.4593D+00   6.0600D+00   2.7521D+00   2.5270D+00   5.2246D+00
  2.1718D-01   1.9872D-05   1.6888D-07   5.9222D-08   3.6356D-05   1.0945D-07   3.3215D-13   2.8269D-10   1.0286D-05   5.4328D-13
  1.0012D+01   1.0561D+01   1.0298D+01   8.2276D+00   8.0392D+00   5.4513D+00   6.0629D+00   2.7350D+00   2.5213D+00   5.3160D+00
  2.1181D+00   2.6699D-05   1.7165D-07   5.8257D-08   4.3248D-05   1.1312D-07   2.6339D-13   2.4412D-10   1.1120D-05   4.2160D-13
  1.0046D+01   1.0636D+01   1.0426D+01   8.2346D+00   8.0535D+00   5.3876D+00   6.0842D+00   2.6249D+00   2.4206D+00   5.4370D+00
  1.8619D+01   2.9393D-05   1.6609D-07   6.0198D-08   4.5791D-05   1.0558D-07   1.9799D-13   1.9830D-10   1.0799D-05   3.1599D-13
  1.0033D+01   1.0661D+01   1.0468D+01   8.2203D+00   8.0236D+00   5.2973D+00   6.0400D+00   2.4997D+00   2.2966D+00   5.4931D+00
  1.2092D+02   2.9213D-05   1.5034D-07   6.6488D-08   4.5897D-05   8.3511D-08   1.0841D-13   1.2505D-10   9.3140D-06   1.7980D-13
  9.9691D+00   1.0662D+01   1.0466D+01   8.1771D+00   7.9217D+00   5.0971D+00   5.8948D+00   2.2425D+00   2.0351D+00   5.5338D+00
  5.1563D+02   2.9058D-05   1.2808D-07   7.8030D-08   4.5744D-05   4.9647D-08   3.0422D-14   4.4355D-11   7.3409D-06   4.9139D-14
  9.8657D+00   1.0660D+01   1.0463D+01   8.1075D+00   7.6959D+00   4.6469D+00   5.5993D+00   1.5914D+00   1.4832D+00   5.6014D+00
  9.9130D+02   2.8905D-05   1.0799D-07   9.2537D-08   4.5575D-05   1.4982D-08   2.0300D-13   4.0548D-12   5.3358D-06   3.2835D-15
  9.7272D+00   1.0659D+01   1.0461D+01   8.0334D+00   7.1756D+00   3.6080D+00   5.0049D+00   5.1634D-01   3.0750D-01   5.6734D+00
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2         SCALE  1.0000D-01   *
PSO2         SCALE  1.0000D-01   +
            0                                                0.5                                                1
  3.977D-13 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
  2.500D-01 | *       |         |         |      +  |         |         |         |         |         |         |
  5.000D-01 | *       |         |         |      +  |         |         |         |         |         |         |
  7.500D-01 | *       |         |         |      +  |         |         |         |         |         |         |
  1.000D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  1.250D+00 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
  1.500D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  1.750D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  2.000D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  2.250D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  2.500D+00 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
  2.750D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  3.000D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  3.250D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  3.500D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  3.750D+00 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
  4.000D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  4.250D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  4.500D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  4.750D+00 | *       |         |         |      +  |         |         |         |         |         |         |
  5.000D+00 |*--------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
  5.250D+00 |*        |         |         |      +  |         |         |         |         |         |         |
  5.500D+00 |*        |         |         |      +  |         |         |         |         |         |         |
  5.750D+00 |*        |         |         |      +  |         |         |         |         |         |         |
  6.000D+00 |*        |         |         |      +  |         |         |         |         |         |         |
  6.250D+00 |*--------|---------|---------|-----+---|---------|---------|---------|---------|---------|---------|
  6.500D+00 |*        |         |         |     +   |         |         |         |         |         |         |
  6.750D+00 |*        |         |         |     +   |         |         |         |         |         |         |
  7.000D+00 |*        |         |         |     +   |         |         |         |         |         |         |
  7.250D+00 |*        |         |         |     +   |         |         |         |         |         |         |
  7.500D+00 |*--------|---------|---------|-----+---|---------|---------|---------|---------|---------|---------|
  7.750D+00 |*        |         |         |     +   |         |         |         |         |         |         |
  8.000D+00 |*        |         |         |     +   |         |         |         |         |         |         |
  8.250D+00 |*        |         |         |     +   |         |         |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2          SCALE  2.0000D+01   A
LO2          SCALE  2.0000D+01   B
LH2O2        SCALE  2.0000D+01   C
            0                                                0.5                                                1
 3.977D-13  |---------|---------|---------|---------|--C------|A-B------|---------|---------|---------|---------|
 2.500D-01  |         |         |         |         |   C     |A B      |         |         |         |         |
 5.000D-01  |         |         |         |         |    C    |A B      |         |         |         |         |
 7.500D-01  |         |         |         |         |     C   |A B      |         |         |         |         |
 1.000D+00  |         |         |         |         |       C A  B      |         |         |         |         |
 1.250D+00  |---------|---------|---------|---------|--------CA--B------|---------|---------|---------|---------|
 1.500D+00  |         |         |         |         |         C  B      |         |         |         |         |
 1.750D+00  |         |         |         |         |         C  B      |         |         |         |         |
 2.000D+00  |         |         |         |         |         AC B      |         |         |         |         |
 2.250D+00  |         |         |         |         |         AC B      |         |         |         |         |
 2.500D+00  |---------|---------|---------|---------|---------AC-B------|---------|---------|---------|---------|
 2.750D+00  |         |         |         |         |         AC B      |         |         |         |         |
 3.000D+00  |         |         |         |         |         AC B      |         |         |         |         |
 3.250D+00  |         |         |         |         |         A CB      |         |         |         |         |
 3.500D+00  |         |         |         |         |         A CB      |         |         |         |         |
 3.750D+00  |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 4.000D+00  |         |         |         |         |         A CB      |         |         |         |         |
 4.250D+00  |         |         |         |         |         A CB      |         |         |         |         |
 4.500D+00  |         |         |         |         |         A CB      |         |         |         |         |
 4.750D+00  |         |         |         |         |         A CB      |         |         |         |         |
 5.000D+00  |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 5.250D+00  |         |         |         |         |         A CB      |         |         |         |         |
 5.500D+00  |         |         |         |         |         A CB      |         |         |         |         |
 5.750D+00  |         |         |         |         |         A CB      |         |         |         |         |
 6.000D+00  |         |         |         |         |         A CB      |         |         |         |         |
 6.250D+00  |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 6.500D+00  |         |         |         |         |         A CB      |         |         |         |         |
 6.750D+00  |         |         |         |         |        A| CB      |         |         |         |         |
 7.000D+00  |         |         |         |         |        A| CB      |         |         |         |         |
 7.250D+00  |         |         |         |         |        A| CB      |         |         |         |         |
 7.500D+00  |---------|---------|---------|---------|--------A|-CB------|---------|---------|---------|---------|
 7.750D+00  |         |         |         |         |        A| CB      |         |         |         |         |
 8.000D+00  |         |         |         |         |        A| CB      |         |         |         |         |
 8.250D+00  |         |         |         |         |        A| CB      |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 10
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+          SCALE  1.00000D+01   A
LO2-         SCALE  1.00000D+01   B
LOH          SCALE  1.00000D+01   C
LOH-         SCALE  1.00000D+01   D
LHO2         SCALE  1.00000D+01   E
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM 11
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-          SCALE  1.00000D+01   A
LH           SCALE  1.00000D+01   B
LHO2-        SCALE  1.00000D+01   C
           0                                                0.5                                                1
 3.977D-13 |---------|---------|----B--A-|----C----|---------|---------|---------|---------|---------|---------|
 2.500D-01 |         |         |    B  A |       C |         |         |         |         |         |         |
 5.000D-01 |         |         |    B  A |         C         |         |         |         |         |         |
 7.500D-01 |         |         |    B  A |         |  C      |         |         |         |         |         |
 1.000D+00 |         |         |    B  A |         |    C    |         |         |         |         |         |
 1.250D+00 |---------|---------|----B--A-|---------|------C--|---------|---------|---------|---------|---------|
 1.500D+00 |         |         |    B  A |         |        C|         |         |         |         |         |
 1.750D+00 |         |         |    B  A |         |         |C        |         |         |         |         |
 2.000D+00 |         |         |    B  A |         |         | C       |         |         |         |         |
 2.250D+00 |         |         |    B A  |         |         |  C      |         |         |         |         |
 2.500D+00 |---------|---------|----B-A--|---------|---------|--C------|---------|---------|---------|---------|
 2.750D+00 |         |         |    B A  |         |         |  C      |         |         |         |         |
 3.000D+00 |         |         |    B A  |         |         |  C      |         |         |         |         |
 3.250D+00 |         |         |    B A  |         |         |  C      |         |         |         |         |
 3.500D+00 |         |         |    B A  |         |         |   C     |         |         |         |         |
 3.750D+00 |---------|---------|----B-A--|---------|---------|---C-----|---------|---------|---------|---------|
 4.000D+00 |         |         |   B A   |         |         |   C     |         |         |         |         |
 4.250D+00 |         |         |   B A   |         |         |    C    |         |         |         |         |
 4.500D+00 |         |         |   B A   |         |         |    C    |         |         |         |         |
 4.750D+00 |         |         |  B A    |         |         |    C    |         |         |         |         |
 5.000D+00 |---------|---------|--B-A----|---------|---------|----C----|---------|---------|---------|---------|
 5.250D+00 |         |         | B A     |         |         |    C    |         |         |         |         |
 5.500D+00 |         |         | B A     |         |         |    C    |         |         |         |         |
 5.750D+00 |         |         |B A      |         |         |    C    |         |         |         |         |
 6.000D+00 |         |         B A       |         |         |    C    |         |         |         |         |
 6.250D+00 |---------|--------B|A--------|---------|---------|----C----|---------|---------|---------|---------|
 6.500D+00 |         |       B A         |         |         |     C   |         |         |         |         |
 6.750D+00 |         |     B  A|         |         |         |     C   |         |         |         |         |
 7.000D+00 |         |    B A  |         |         |         |     C   |         |         |         |         |
 7.250D+00 |         |  B A    |         |         |         |     C   |         |         |         |         |
 7.500D+00 |--------B|A--------|---------|---------|---------|-----C---|---------|---------|---------|---------|
 7.750D+00 |    B A  |         |         |         |         |      C  |         |         |         |         |
 8.000D+00 |  B A    |         |         |         |         |      C  |         |         |         |         |
 8.250D+00 |  B A    |         |         |         |         |      C  |         |         |         |         |
```

```
PRINT STREAM NO.  2
  DOMR        H2O2        H+          OH-         PSO2        O2-         H           OH          PSH2        E-
  2.1789D-03  3.2158D-06  1.6724D-07  5.9825D-08  3.6900D-02  1.0738D-07  3.0757D-13  2.9709D-10  2.0900D-03  5.8445D-13
  2.1782D-02  1.6064D-05  1.6850D-07  5.9362D-08  3.6899D-02  1.0897D-07  3.3650D-13  2.8792D-10  2.0897D-03  5.6512D-13
  2.1718D-01  1.9872D-05  1.6888D-07  5.9222D-08  3.6879D-02  1.0945D-07  3.3219D-13  2.8269D-10  2.0850D-03  5.4329D-13
  2.1181D+00  2.6699D-05  1.7165D-07  5.8256D-08  3.6770D-02  1.1312D-07  2.6364D-13  2.4409D-10  2.0497D-03  4.2175D-13
  1.8619D+01  2.9396D-05  1.6610D-07  6.0193D-08  3.6646D-02  1.0560D-07  1.9867D-13  1.9820D-10  1.8757D-03  3.1634D-13
  1.2092D+02  2.9173D-05  1.5033D-07  6.6495D-08  3.6460D-02  8.3490D-08  1.0863D-13  1.2515D-10  1.5178D-03  1.7508D-13
  5.1564D+02  2.8988D-05  1.2806D-07  7.8038D-08  3.6289D-02  4.9628D-08  3.0503D-14  4.4425D-11  1.1889D-03  4.9261D-14
  9.9130D+02  2.8805D-05  1.0799D-07  9.2540D-08  3.6119D-02  1.4979D-08  2.0372D-15  4.0667D-12  8.6202D-04  3.2948D-15
```

FIG. I-2

$f_{Zr-H_2O} = 0.00612$

```
PRINT STREAM NO.  3
  DOMR         HO2          H2O          HO2-         PO2          PH2          PSO2         PSH2
  2.1789D-03   1.1227D-09   5.5300D+01   3.3845D-11   4.0953D-02   2.3195D-03   3.6900D-02   2.0900D-03
  2.1782D-02   1.1480D-09   5.5300D+01   1.6773D-10   4.0951D-02   2.3193D-03   3.6899D-02   2.0897D-03
  2.1718D-01   1.1558D-09   5.5300D+01   2.0700D-10   4.0929D-02   2.3140D-03   3.6879D-02   2.0850D-03
  2.1181D+00   1.2142D-09   5.5300D+01   2.7355D-10   4.0809D-02   2.2748D-03   3.6770D-02   2.0497D-03
  1.8619D+01   1.0967D-09   5.5300D+01   3.1126D-10   4.0671D-02   2.0817D-03   3.6646D-02   1.8757D-03
  1.2092D+02   7.8468D-10   5.5300D+01   3.4142D-10   4.0464D-02   1.6845D-03   3.6460D-02   1.5178D-03
  5.1554D+02   3.9730D-10   5.5301D+01   3.9845D-10   4.0274D-02   1.3195D-03   3.6289D-02   1.1889D-03
  9.9130D+02   1.0110D-10   5.5301D+01   4.6985D-10   4.0085D-02   9.5670D-04   3.6119D-02   8.6202D-04
```

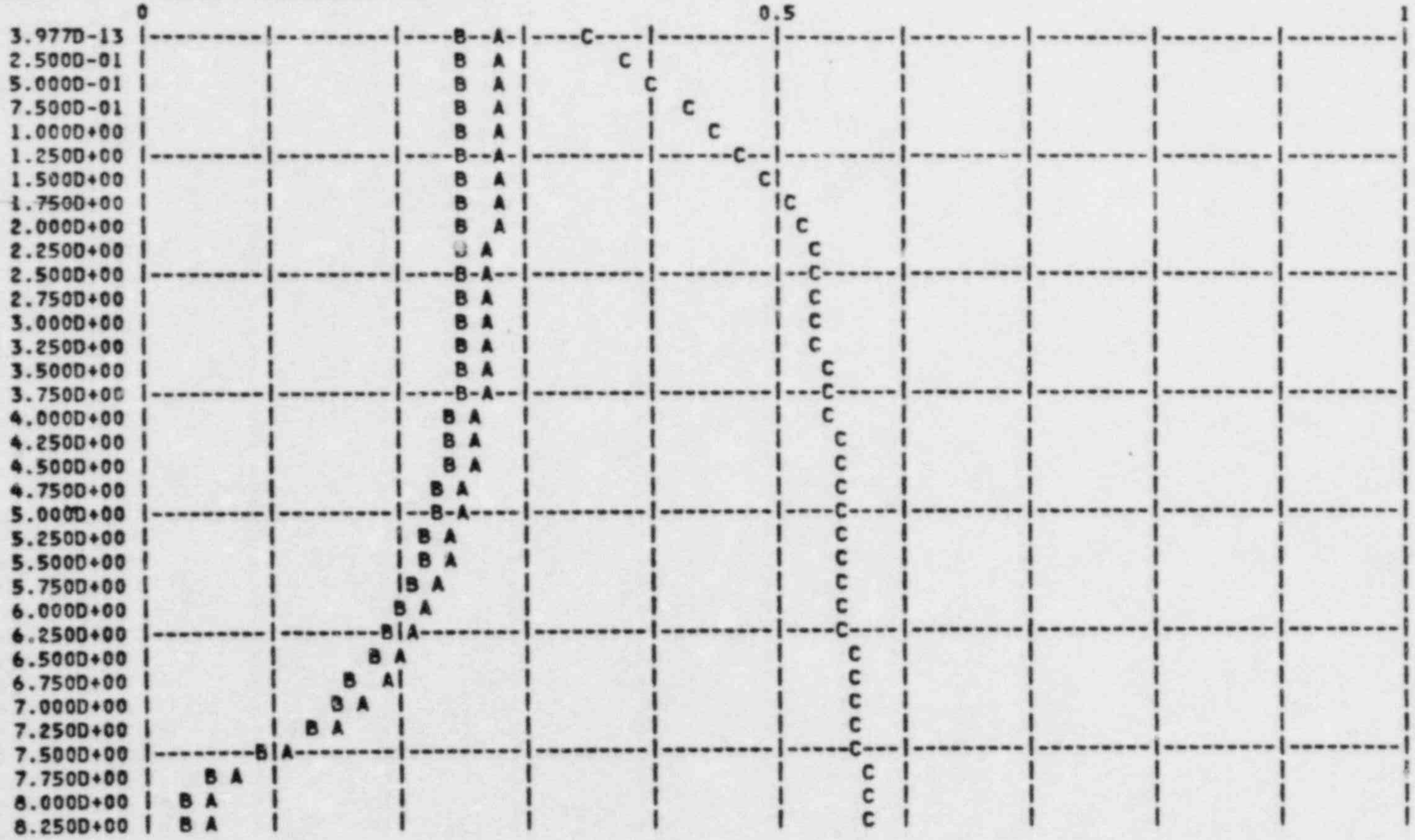
```
PRINT STREAM NO.  6
  DOMR         H2O2         H+           OH-          O2           O2-          H            OH           H2           E-
  LH2          LO2          LH2O2        LH+          LO2-         LOH          LHO2         LE-          LH           LHO2-
  2.1789D-03   3.2158D-06   1.6724D-07   5.9825D-08   4.4520D-05   1.0738D-07   3.0757D-13   2.9709D-10   1.2515D-05   5.8445D-13
. 1.0097D+01   1.0649D+01   9.5073D+00   8.2233D+00   8.0309D+00   5.4729D+00   6.0503D+00   2.7667D+00   2.4879D+00   4.5295D+00
  2.1782D-02   1.6064D-05   1.6850D-07   5.9362D-08   3.7305D-05   1.0897D-07   3.3650D-13   2.8792D-10   1.0884D-05   5.6512D-13
  1.0037D+01   1.0572D+01   1.0206D+01   8.2266D+00   8.0373D+00   5.4593D+00   6.0600D+00   2.7521D+00   2.5270D+00   5.2246D+00
  2.1718D-01   1.9872D-05   1.6888D-07   5.9222D-08   3.6355D-05   1.0945D-07   3.3219D-13   2.8269D-10   1.0287D-05   5.4329D-13
  1.0012D+01   1.0561D+01   1.0298D+01   8.2276D+00   8.0392D+00   5.4513D+00   6.0629D+00   2.7350D+00   2.5214D+00   5.3160D+00
  2.1181D+00   2.6699D-05   1.7165D-07   5.8256D-08   4.3226D-05   1.1312D-07   2.6364D-13   2.4409D-10   1.1133D-05   4.2175D-13
  1.0047D+01   1.0636D+01   1.0426D+01   8.2347D+00   8.0536D+00   5.3876D+00   6.0843D+00   2.6251D+00   2.4210D+00   5.4370D+00
  1.8619D+01   2.9396D-05   1.6610D-07   6.0193D-08   4.5715D-05   1.0560D-07   1.9867D-13   1.9820D-10   1.0847D-05   3.1634D-13
  1.0035D+01   1.0660D+01   1.0468D+01   8.2204D+00   8.0237D+00   5.2971D+00   6.0401D+00   2.5001D+00   2.2981D+00   5.4931D+00
  1.2092D+02   2.9173D-05   1.5033D-07   6.6495D-08   4.5819D-05   8.3490D-08   1.0863D-13   1.2515D-10   9.3136D-06   1.7500D-13
  9.9691D+00   1.0661D+01   1.0465D+01   8.1770D+00   7.9216D+00   5.0974D+00   5.8947D+00   2.2432D+00   2.0359D+00   5.5333D+00
  5.1564D+02   2.8988D-05   1.2806D-07   7.8036D-08   4.5628D-05   4.9628D-08   3.0503D-14   4.4425D-11   7.3312D-06   4.9261D-14
  9.8652D+00   1.0659D+01   1.0462D+01   8.1074D+00   7.6957D+00   4.6476D+00   5.5991D+00   1.6925D+00   1.4843D+00   5.6004D+00
  9.9130D+02   2.8805D-05   1.0799D-07   9.2540D-08   4.5417D-05   1.4979D-08   2.0372D-15   4.0667D-12   5.3206D-06   3.2948D-15
  9.7260D+00   1.0657D+01   1.0459D+01   8.0334D+00   7.1755D+00   3.6092D+00   5.0048D+00   5.1783D-01   3.0903D-01   5.6720D+00
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG    (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2         SCALE  1.00000D-01  *
PSO2         SCALE  1.00000D-01  +
           0                                                0.5                                                1
 3.977D-13 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
 2.500D-01 | *       |         |         |      +  |         |         |         |         |         |         |
 5.000D-01 | *       |         |         |      +  |         |         |         |         |         |         |
 7.500D-01 | *       |         |         |      +  |         |         |         |         |         |         |
 1.000D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 1.250D+00 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
 1.500D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 1.750D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 2.000D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 2.250D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 2.500D+00 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
 2.750D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 3.000D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 3.250D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 3.500D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 3.750D+00 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
 4.000D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 4.250D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 4.500D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 4.750D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 5.000D+00 |-*-------|---------|---------|------+--|---------|---------|---------|---------|---------|---------|
 5.250D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 5.500D+00 | *       |         |         |      +  |         |         |         |         |         |         |
 5.750D+00 | *       |         |         |     +   |         |         |         |         |         |         |
 6.000D+00 | *       |         |         |     +   |         |         |         |         |         |         |
 6.250D+00 |*--------|---------|---------|-----+---|---------|---------|---------|---------|---------|---------|
 6.500D+00 |*        |         |         |     +   |         |         |         |         |         |         |
 6.750D+00 |*        |         |         |     +   |         |         |         |         |         |         |
 7.000D+00 |*        |         |         |     +   |         |         |         |         |         |         |
 7.250D+00 |*        |         |         |     +   |         |         |         |         |         |         |
 7.500D+00 |*--------|---------|---------|-----+---|---------|---------|---------|---------|---------|---------|
 7.750D+00 |*        |         |         |     +   |         |         |         |         |         |         |
 8.000D+00 |*        |         |         |     +   |         |         |         |         |         |         |
 8.250D+00 |*        |         |         |     +   |         |         |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2          SCALE  2.00000D+01   A
LO2          SCALE  2.00000D+01   B
LH2O2        SCALE  2.00000D+01   C
           0                                                0.5                                                1
 3.977D-13 |---------|---------|---------|---------|--C------|A-B------|---------|---------|---------|---------|
 2.500D-01 |         |         |         |         |   C     |A B      |         |         |         |         |
 5.000D-01 |         |         |         |         |    C    |A B      |         |         |         |         |
 7.500D-01 |         |         |         |         |     C   |A B      |         |         |         |         |
 1.000D+00 |         |         |         |         |       C A  B      |         |         |         |         |
 1.250D+00 |---------|---------|---------|---------|--------CA--B------|---------|---------|---------|---------|
 1.500D+00 |         |         |         |         |         C  B      |         |         |         |         |
 1.750D+00 |         |         |         |         |         C  B      |         |         |         |         |
 2.000D+00 |         |         |         |         |         AC B      |         |         |         |         |
 2.250D+00 |         |         |         |         |         AC B      |         |         |         |         |
 2.500D+00 |---------|---------|---------|---------|---------AC-B------|---------|---------|---------|---------|
 2.750D+00 |         |         |         |         |         AC B      |         |         |         |         |
 3.000D+00 |         |         |         |         |         AC B      |         |         |         |         |
 3.250D+00 |         |         |         |         |         A CB      |         |         |         |         |
 3.500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 3.750D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 4.000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 4.250D+00 |         |         |         |         |         A CB      |         |         |         |         |
 4.500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 4.750D+00 |         |         |         |         |         A CB      |         |         |         |         |
 5.000D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 5.250D+00 |         |         |         |         |         A CB      |         |         |         |         |
 5.500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 5.750D+00 |         |         |         |         |         A CB      |         |         |         |         |
 6.000D+00 |         |         |         |         |         A CB      |         |         |         |         |
 6.250D+00 |---------|---------|---------|---------|---------A-CB------|---------|---------|---------|---------|
 6.500D+00 |         |         |         |         |         A CB      |         |         |         |         |
 6.750D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.250D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 7.500D+00 |---------|---------|---------|---------|--------A|-CB------|---------|---------|---------|---------|
 7.750D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 8.000D+00 |         |         |         |         |        A| CB      |         |         |         |         |
 8.250D+00 |         |         |         |         |        A| CB      |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 10
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+          SCALE  1.0000D+01   A
LO2-         SCALE  1.0000D+01   B
LOH          SCALE  1.0000D+01   C
LOH-         SCALE  1.0000D+01   D
LHO2         SCALE  1.0000D+01   E
          0                                                0.5                                                1
3.977D-13 |---------|---------|---------|---------|---------|----C----E---------|-------D-B-A-------|---------|
2.500D-01 |         |         |         |         |         |    C    E         |       D B A       |         |
5.000D-01 |         |         |         |         |         |    C    E         |       D B A       |         |
7.500D-01 |         |         |         |         |         |    C    E         |       D B A       |         |
1.000D+00 |         |         |         |         |         |    C    |E        |       D B A       |         |
1.250D+00 |---------|---------|---------|---------|---------|----C----|E--------|-------D-B-A-------|---------|
1.500D+00 |         |         |         |         |         |    C    |E        |       D B A       |         |
1.750D+00 |         |         |         |         |         |    C    |E        |       D B A       |         |
2.000D+00 |         |         |         |         |         |    C    |E        |       D B A       |         |
2.250D+00 |         |         |         |         |         |    C    |E        |       D B A       |         |
2.500D+00 |---------|---------|---------|---------|---------|----C----|E--------|-------D-B-A-------|---------|
2.750D+00 |         |         |         |         |         |    C    |E        |       D B A       |         |
3.000D+00 |         |         |         |         |         |    C    |E        |       D B A       |         |
3.250D+00 |         |         |         |         |         |   C     |E        |       D B A       |         |
3.500D+00 |         |         |         |         |         |   C     |E        |       D B A       |         |
3.750D+00 |---------|---------|---------|---------|---------|---C-----|E--------|-------D-|BA-------|---------|
4.000D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
4.250D+00 |         |         |         |         |         |   C     |E        |       D |BA       |         |
4.500D+00 |         |         |         |         |         |  C      |E        |       D B A       |         |
4.750D+00 |         |         |         |         |         |  C      |E        |       D B A       |         |
5.000D+00 |---------|---------|---------|---------|---------|--C------E---------|-------D-B-A-------|---------|
5.250D+00 |         |         |         |         |         |  C      E         |       D B A       |         |
5.500D+00 |         |         |         |         |         | C       E         |       D B A       |         |
5.750D+00 |         |         |         |         |         | C      E|         |       DB| A       |         |
6.000D+00 |         |         |         |         |         |C       E|         |       DB| A       |         |
6.250D+00 |---------|---------|---------|---------|---------C-------E-|---------|-------DB|-A-------|---------|
6.500D+00 |         |         |         |         |        C|       E |         |       BD|A        |         |
6.750D+00 |         |         |         |         |       C |      E  |         |       BD|A        |         |
7.000D+00 |         |         |         |         |     C   |     E   |         |     B  D|A        |         |
7.250D+00 |         |         |         |         |    C    |    E    |         |    B   D|A        |         |
7.500D+00 |---------|---------|---------|---------|C--------|--E------|---------|---B----D|A--------|---------|
7.750D+00 |         |         |         |       C |         |E        |         |  B      D         |         |
8.000D+00 |         |         |         |     C   |         E         |         | B       D         |         |
8.250D+00 |         |         |         |     C   |         E         |         | B       D         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 11
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEFENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-          SCALE  1.0000D+01   A
LH           SCALE  1.0000D+01   B
LHO2-        SCALE  1.0000D+01   C
```



APPENDIX J

SENSITIVITY ANALYSIS OF TEMPERATURE EFFECTS ON CHEMICAL KINETIC RATE CONSTANTS AND GAS SOLUBILITY

This Appendix documents the results of the sensitivity of the BASE CASE results to temperature. Figure J-1 is a listing of a short computer program utilized to extrapolate the chemical kinetics rate constants for various temperatures (25°C, 50°C, 75°C, and 100°C) based on Arrhenius' Law. The thirty-one constants evaluated corresponds to the chemical reactions shown in Figure XVI of Section 4.1.2 in Volume I. Figure J-2 is a listing of the results of the temperature extrapolations. The temperature effects on solubility of H_2 and O_2 gas in containment can be extracted from calculations carried out in Appendix F. Figure J-3 is the FACSIMILE simulation of Radiolysis/ Recombination at T=100°C.

```
FORTRAN IV G LEVEL  21                MAIN                DATE = 82165          15/57/28                PAGE 0001
               C                                                                        00000050
               C     CALCULATION OF TEMPERATURE EFFECTS ON                              00000060
               C     CHEMICAL KINETIC RATE CONSTANTS                                    00000070
               C             JOHN BICKEL                                                00000080
               C            JUNE 14, 1982                                               00000090
               C                                                                        00000100
               C ********************************************************************  00000110
               C                                                                        00000120
 0001                DIMENSION CK(31), TC(4), TK(4), TF(4), EA(31), X(4)                00000130
 0002                REAL * 8 CK, TC, TK, TF, EA, X, R                                  00000140
               C                                                                        00000150
               C ********************************************************************  00000160
 0003                DATA CK /1.6D1,2.4D10,3.0D10,1.3D10,1.0D10,2.0D10,1.9D10,          00000170
                    X        1.64D6, 4.5D9, 1.2D10, 1.2D10, 2.0D7, 4.5D8, 6.3D7,        00000180
                    X        1.4378D11, 2.6D-5, 2.0D10, 4.5D7,4.5D7, 9.0D7, 1.9D10,     00000190
                    X        8.0D5, 5.0D10, 1.5D7, 2.7D6, 5.6D3, 2.0D10, 2.0D10,        00000200
                    X        3.3D6, 1.0D8, 1.022D4/                                     00000210
               C                                                                        00000220
               C     CORRESPONDING ACTIVATION ENERGIES IN CAL./MOLE                     00000230
               C                                                                        00000240
 0004                DATA EA/ 3.0D3, 3.0D3, 3.0D3, 3.0D3, 3.0D3, 3.0D3, 3.0D3, 3.0D3,   00000250
                    X         3.0D3, 3.0D3, 3.0D3, 3.0D3, 3.0D3, 3.0D3, 3.0D3, 3.0D3,   00000260
                    X         3.0D3, 7.0D3, 4.5D3, 4.5D3, 3.0D3, 3.0D3, 3.0D3, 4.5D3,   00000270
                    X         4.5D3, 4.5D3, 3.0D3, 3.0D3, 4.5D3, 4.5D3, 3.0D3/          00000280
               C                                                                        00000290
               C     TEMPERATURE DATA IN DEGREES CENTIGRADE                             00000300
               C                                                                        00000310
 0005                DATA TC/ 2.5D1, 5.0D1, 7.5D1, 1.0D2/                               00000320
               C                                                                        00000330
               C     CONVERT TEMPERATURE FROM CENTIGRADE TO KELVIN, FAHRENHEIT          00000340
               C                                                                        00000350
 0006                DO 5 I = 1,4                                                       00000360
 0007                TK(I) = 2.7315D2 + TC(I)                                           00000370
 0008              5 TF(I) = 3.2D1 + 1.8D0 * TC(I)                                      00000380
 0009                R = 8.205D-2                                                       00000390
               C                                                                        00000400
               C     EXTRAPOLATE RATE CONSTANTS VIA ARREHNIUS' LAW                      00000410
               C                                                                        00000420
 0010                DO 50 L = 1,31                                                     00000430
 0011                X(1) = CK(L)                                                       00000440
 0012                DO 25 M = 2,4,1                                                    00000450
 0013             25 X(M) = CK(L) * DEXP((-4.1311D-2 * EA(L) / R) *((1.0D0 / TK(M)) -   00000460
                    X (1.0D0/TK(1))))                                                   00000470
 0014                DO 27 N = 1,4                                                      00000471
 0015             27 WRITE (6,30) TC(N), TK(N), TF(N), L, X(N)                          00000480
 0016             30 FORMAT('0','TEMPERATURE =',D10.3,' DEG.C =',D10.3,' DEG.K =',      00000490
                    X D10.3,'DEG.F',2X,'K(',I2,') =',D10.3)                             00000500
 0017             50 CONTINUE                                                           00000510
 0018                STOP                                                               00000520
 0019                END                                                                00000530
```

FIG. J-1

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 1) = 0.160D 02
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 1) = 0.237D 02
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 1) = 0.331D 02
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 1) = 0.443D 02
```

$e_{aq}^- + H_2O \rightarrow H + OH^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 2) = 0.240D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 2) = 0.355D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 2) = 0.497D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 2) = 0.664D 11
```

$e_{aq}^- + H^+ \rightarrow H$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 3) = 0.300D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 3) = 0.444D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 3) = 0.621D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 3) = 0.830D 11
```

$e_{aq}^- + OH \rightarrow OH^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 4) = 0.130D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 4) = 0.192D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 4) = 0.269D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 4) = 0.360D 11
```

$e_{aq}^- + H_2O_2 \rightarrow OH + OH^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 5) = 0.100D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 5) = 0.148D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 5) = 0.207D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 5) = 0.277D 11
```

$H + H \rightarrow H_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 6) = 0.200D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 6) = 0.296D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 6) = 0.414D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 6) = 0.554D 11
```

$e_{aq}^- + HO_2 \rightarrow HO_2^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 7) = 0.190D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 7) = 0.281D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 7) = 0.393D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 7) = 0.526D 11
```

$e_{aq}^- + O_2 \rightarrow O_2^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 8) = 0.164D 07
```

$2e_{aq}^- + 2H_2O \rightarrow 2OH^- + H_2$

FIG. J-2

```
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 8) = 0.243D 07
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 8) = 0.339D 07
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 8) = 0.434D 07
```

$2e_{aq}^- + 2H_2O \rightarrow 2OH^- + H_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K( 9) = 0.450D 10
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K( 9) = 0.666D 10
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K( 9) = 0.932D 10
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K( 9) = 0.125D 11
```

$2OH \rightarrow H_2O_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(10) = 0.120D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(10) = 0.178D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(10) = 0.248D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(10) = 0.332D 11
```

$OH + HO_2 \rightarrow H_2O + O_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(11) = 0.120D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(11) = 0.178D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(11) = 0.248D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(11) = 0.332D 11
```

$OH + O_2^- \rightarrow OH^- + O_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(12) = 0.200D 08
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(12) = 0.296D 08
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(12) = 0.414D 08
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(12) = 0.554D 08
```

$OH^- + H \rightarrow e_{aq}^- + H_2O$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(13) = 0.450D 09
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(13) = 0.666D 09
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(13) = 0.932D 09
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(13) = 0.125D 10
```

$e_{aq}^- + H + H_2O \rightarrow OH^- + H_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(14) = 0.630D 08
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(14) = 0.932D 08
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(14) = 0.130D 09
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(14) = 0.174D 09
```

$e_{aq}^- + HO_2^- + H_2O \rightarrow OH + 2OH^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(15) = 0.144D 12
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(15) = 0.213D 12
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(15) = 0.298D 12
```

$H^+ + OH^- \rightarrow H_2O$

```
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(15) = 0.398D 12
```

$H^+ + OH^- \rightarrow H_2O$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(16) = 0.260D-04
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(16) = 0.385D-04
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(16) = 0.538D-04
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(16) = 0.720D-04
```

$H_2O \rightarrow H^+ + OH^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(17) = 0.200D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(17) = 0.296D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(17) = 0.414D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(17) = 0.554D 11
```

$H + OH \rightarrow H_2O$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(18) = 0.450D 08
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(18) = 0.112D 09
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(18) = 0.246D 09
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(18) = 0.484D 09
```

$OH + H_2 \rightarrow H + H_2O$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(19) = 0.450D 08
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(19) = 0.810D 08
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(19) = 0.134D 09
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(19) = 0.207D 09
```

$OH + H_2O_2 \rightarrow H_2O + HO_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(20) = 0.900D 08
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(20) = 0.162D 09
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(20) = 0.268D 09
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(20) = 0.415D 09
```

$H + H_2O_2 \rightarrow OH + H_2O$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(21) = 0.190D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(21) = 0.281D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(21) = 0.393D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(21) = 0.526D 11
```

$H + O_2 \rightarrow HO_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(22) = 0.800D 06
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(22) = 0.118D 07
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(22) = 0.166D 07
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(22) = 0.221D 07
```

$HO_2 \rightarrow O_2^- + H^+$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(23) = 0.500D 11
```

$O_2^- + H^+ \rightarrow HO_2$

```
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(23) = 0.740D 11
TEMPERATURE = 0.750D 02 DEG.C - 0.348D 03 DEG.K = 0.167D 03DEG.F  K(23) = 0.104D 12
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(23) = 0.138D 12
```

$O_2^{\cdot -} + H^+ \rightarrow HO_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(24) = 0.150D 08
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(24) = 0.270D 08
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(24) = 0.447D 08
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(24) = 0.691D 08
```

$HO_2 + O_2^- \rightarrow O_2 + HO_2^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(25) = 0.270D 07
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(25) = 0.486D 07
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(25) = 0.804D 07
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(25) = 0.124D 08
```

$2HO_2 \rightarrow H_2O_2 + O_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(26) = 0.560D 04
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(26) = 0.101D 05
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(26) = 0.167D 05
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(26) = 0.258D 05
```

$2O_2^- + 2H_2O \rightarrow H_2O_2 + O_2 + 2OH^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(27) = 0.200D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(27) = 0.296D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(27) = 0.414D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(27) = 0.554D 11
```

$H + HO_2 \rightarrow H_2O_2$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(28) = 0.200D 11
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(28) = 0.296D 11
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(28) = 0.414D 11
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(28) = 0.554D 11
```

$H + O_2^- \rightarrow HO_2^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(29) = 0.330D 07
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(29) = 0.594D 07
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(29) = 0.983D 07
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(29) = 0.152D 08
```

$e_{aq}^- + O_2^- + H_2O \rightarrow HO_2^- + OH^-$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(30) = 0.100D 09
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(30) = 0.180D 09
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(30) = 0.298D 09
```

$OH^- + H_2O_2 \rightarrow HO_2^- + H_2O$

```
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(30) = 0.461D 09
```

$OH^- + H_2O_2 \rightarrow HO_2^- + H_2O$

```
TEMPERATURE = 0.250D 02 DEG.C = 0.298D 03 DEG.K = 0.770D 02DEG.F  K(31) = 0.102D 05
TEMPERATURE = 0.500D 02 DEG.C = 0.323D 03 DEG.K = 0.122D 03DEG.F  K(31) = 0.151D 05
TEMPERATURE = 0.750D 02 DEG.C = 0.348D 03 DEG.K = 0.167D 03DEG.F  K(31) = 0.212D 05
TEMPERATURE = 0.100D 03 DEG.C = 0.373D 03 DEG.K = 0.212D 03DEG.F  K(31) = 0.283D 05
```

$HO_2^- + H_2O \rightarrow OH^- + H_2O_2$

```
PRINT STREAM NO.  2
  DOMR        H2O2        H+          OH-         PSO2        O2-         H           OH          PSH2        E-
  2.1789D-03  6.4847D-06  1.4999D-07  6.6695D-08  5.1300D-02  8.3224D-08  3.4582D-13  3.3760D-11  4.2400D-02  2.5128D-13
  2.1782D-02  2.1956D-05  1.4705D-07  6.7967D-08  5.1295D-02  7.8823D-08  5.2167D-13  9.3050D-11  4.2395D-02  3.3120D-13
  2.1718D-01  1.4070D-05  1.4475D-07  6.9079D-08  5.1241D-02  7.5499D-08  3.2002D-13  1.3834D-10  4.2318D-02  3.5605D-13
  2.1181D+00  1.9219D-05  1.4502D-07  6.8925D-08  5.0783D-02  7.5864D-06  2.4157D-13  1.0514D-10  4.1563D-02  2.6213D-13
  1.8622D+01  2.1565D-05  1.4049D-07  7.1132D-08  4.7414D-02  6.9092D-08  1.7932D-13  7.8484D-11  3.4892D-02  1.9172D-13
  1.2092D+02  1.7032D-05  1.2908D-07  7.7454D-08  3.3621D-02  5.1398D-08  8.2095D-14  5.8274D-11  7.2681D-03  1.1577D-13
  5.1564D+02  1.5237D-05  1.1510D-07  8.6859D-08  3.0737D-02  2.8008D-08  2.0987D-14  1.9783D-11  1.4802D-03  3.3729D-14
  9.9123D+02  1.5193D-05  1.0394D-07  9.6179D-08  3.0680D-02  7.5014D-09  1.3983D-15  1.4218D-12  1.3671D-03  2.2492D-15
```

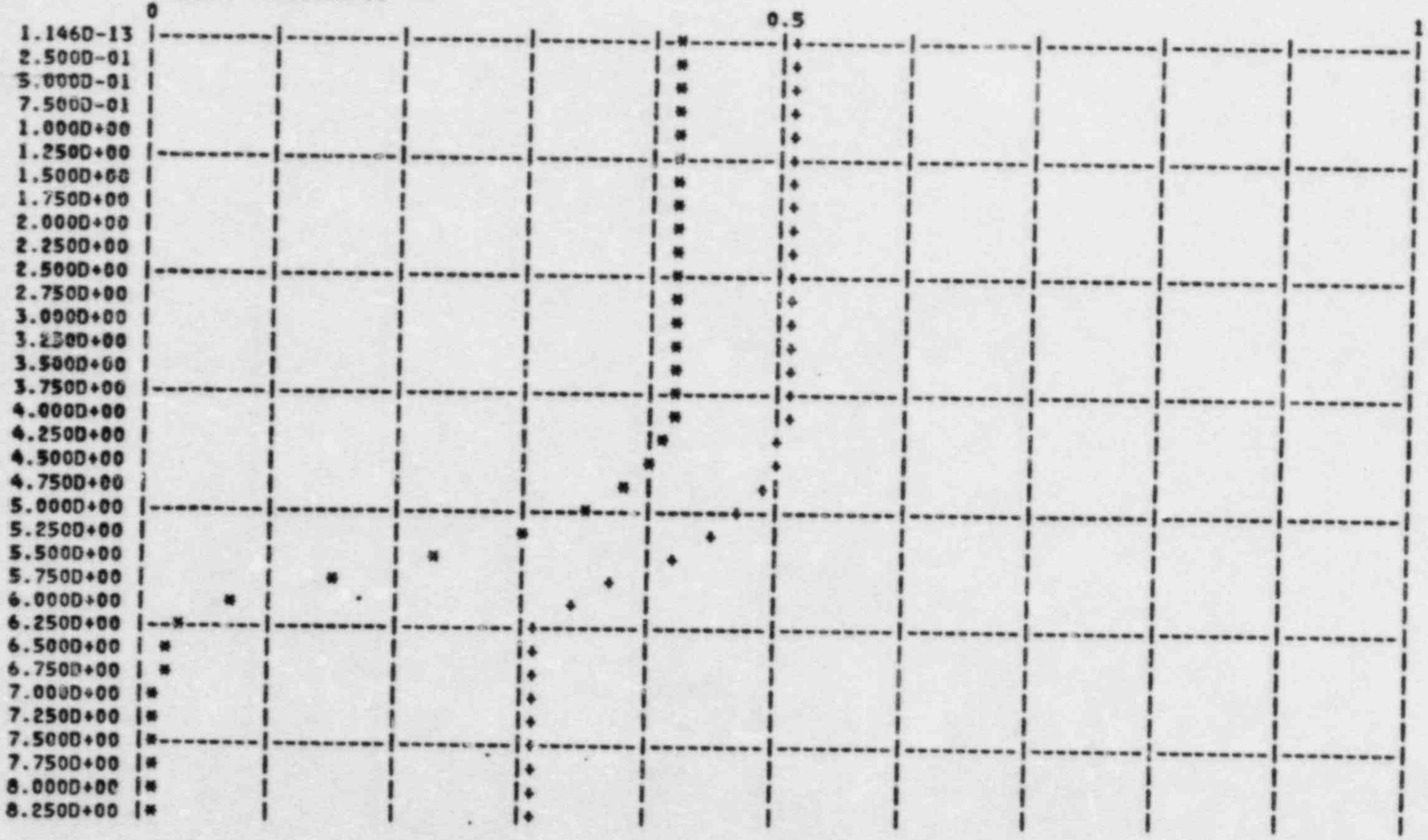
FIG. J-3

```
PRINT STREAM NO.  3
  DOMR        HO2         H2O         HO2-        PO2         PH2         PSO2        PSH2
  2.1789D-03  7.8103D-10  5.5300D+01  7.5427D-11  4.5491D-02  3.7599D-02  5.1300D-02  4.2400D-02
  2.1782D-02  7.2546D-10  5.5300D+01  2.6030D-10  4.5487D-02  3.7595D-02  5.1295D-02  4.2395D-02
  2.1718D-01  6.8389D-10  5.5300D+01  1.6957D-10  4.5438D-02  3.7526D-02  5.1241D-02  4.2318D-02
  2.1181D+00  6.8849D-10  5.5301D+01  2.3110D-10  4.5033D-02  3.6856D-02  5.0783D-02  4.1563D-02
  1.8622D+01  6.0740D-10  5.5307D+01  2.6770D-10  4.2045D-02  3.0941D-02  4.7414D-02  3.4892D-02
  1.2092D+02  4.1505D-10  5.5331D+01  2.3037D-10  2.9814D-02  6.4450D-03  3.3621D-02  7.2681D-03
  5.1564D+02  2.0159D-10  5.5336D+01  2.3140D-10  2.7256D-02  1.3126D-03  3.0737D-02  1.4802D-03
  9.9123D+02  4.8737D-11  5.5337D+01  2.5577D-10  2.7206D-02  1.2123D-03  3.0680D-02  1.3671D-03
```

```
PRINT STREAM NO.  4
  DOMR          TIME          H2T           O2T           H2O2T
  2.1789D-03   1.0000D+01   3.4400D-04   3.9299D-04   7.8781D-08
  2.1782D-02   1.0000D+02   3.4395D-04   3.9291D-04   4.1721D-06
  2.1718D-01   1.0000D+03   3.4332D-04   3.9250D-04   3.0543D-05
  2.1181D+00   1.0000D+04   3.3719D-04   3.8901D-04   1.5945D-04
  1.8622D+01   1.0000D+05   2.8307D-04   3.6320D-04   2.1137D-04
  1.2092D+02   1.0000D+06   5.8965D-05   2.5757D-04   1.6704D-04
  5.1564D+02   1.0000D+07   1.2009D-05   2.3547D-04   1.4933D-04
  9.9123D+02   1.0000D+08   1.1092D-05   2.3504D-04   1.4890D-04
```

```
PRINT STREAM NO.  6
  DOMR         H2O2         H+           OH-          O2           O2-          H            OH           H2           E-
  LH2          LO2          LH2O2        LH+          LO2-         LOH          LHO2         LE-          LH           LHO2-
  2.1789D-03 -6.4847D-06  1.4999D-07  6.6695D-08  3.4795D-05  8.3224D-08  3.4582D-13  3.3760D-11  3.1097D-05  2.5128D-13
  1.0493D+01  1.0542D+01  9.8119D+00  8.1761D+00  7.9202D+00  4.5284D+00  5.8927D+00  2.4002D+00  2.5388D+00  4.8775D+00
  2.1782D-02 -2.1956D-05  1.4705D-07  6.7967D-08  1.4667D-05  7.8823D-08  5.2167D-13  9.3050D-11  6.2464D-06  3.3120D-13
  9.7956D+00  1.0166D+01  1.0342D+01  8.1675D+00  7.8967D+00  4.9687D+00  5.8606D+00  2.5201D+00  2.7174D+00  5.4155D+00
  2.1718D-01 -1.4070D-05  1.4475D-07  6.9079D-08  1.7816D-05  7.5499D-08  3.2002D-13  1.3834D-10  2.6200D-06  3.5605D-13
  9.4183D+00  1.0251D+01  1.0148D+01  8.1606D+00  7.8779D+00  5.1409D+00  5.8350D+00  2.5515D+00  2.5052D+00  5.2294D+00
  2.1181D+00 -1.9219D-05  1.4502D-07  6.8925D-08  2.2505D-05  7.5664D-08  2.4157D-13  1.0514D-10  3.3003D-06  2.6213D-13
  9.5186D+00  1.0352D+01  1.0284D+01  8.1614D+00  7.8030D+00  5.0217D+00  5.8379D+00  2.4185D+00  2.3030D+00  5.3638D+00
  1.6622D+01 -2.1565D-05  1.4049D-07  7.1132D-08  2.4404D-05  6.9092D-08  1.7932D-13  7.8484D-11  3.5710D-06  1.9172D-13
  9.5528D+00  1.0387D+01  1.0334D+01  8.1477D+00  7.8394D+00  4.8948D+00  5.7835D+00  2.2827D+00  2.2536D+00  5.4276D+00
  1.2092D+02 -1.7032D-05  1.2908D-07  7.7454D-08  2.4196D-05  5.1398D-08  8.2098D-14  5.8274D-11  1.8345D-06  1.1577D-13
  9.2635D+00  1.0384D+01  1.0231D+01  8.1109D+00  7.7109D+00  4.7655D+00  5.6181D+00  2.0636D+00  1.9143D+00  5.3624D+00
  5.1564D+02 -1.5237D-05  1.1510D-07  8.6859D-08  2.4025D-05  2.8008D-08  2.0987D-14  1.9763D-11  1.2233D-06  3.3729D-14
  9.0875D+00  1.0381D+01  1.0183D+01  8.0611D+00  7.4473D+00  4.2963D+00  5.3045D+00  1.5280D+00  1.3220D+00  5.3644D+00
  9.9123D+02 -1.5193D-05  1.0394D-07  9.6179D-08  2.3982D-05  7.5014D-09  1.3983D-15  1.4218D-12  1.1317D-06  2.2492D-15
  9.0537D+00  1.0380D+01  1.0182D+01  8.0168D+00  6.8751D+00  3.1528D+00  4.6879D+00  3.5202D-01  1.4559D-01  5.4078D+00
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM  8
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
PSH2          SCALE  1.0000D-01   *
PSO2          SCALE  1.0000D-01   +
```



```
PLOTTING PARAMETERS FOR GRAPH STREAM  9
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH2           SCALE  2.0000D+01   A
LO2           SCALE  2.0000D+01   B
LH2O2         SCALE  2.0000D+01   C
          0                                               0.5                                               1
1.146D-13 |---------|---------|---------|---------|---C--- -|--B------|---------|---------|---------|---------|
2.500D-01 |         |         |         |         |    C    |  B      |         |         |         |         |
5.000D-01 |         |         |         |         |      C  |  B      |         |         |         |         |
7.500D-01 |         |         |         |         |       C |  B      |         |         |         |         |
1.000D+00 |         |         |         |         |        C| AB      |         |         |         |         |
1.250D+00 |---------|---------|---------|---------|---------C-B-------|---------|---------|---------|---------|
1.500D+00 |         |         |         |         |         |CB       |         |         |         |         |
1.750D+00 |         |         |         |         |         |BC       |         |         |         |         |
2.000D+00 |         |         |         |         |        A|BC       |         |         |         |         |
2.250D+00 |         |         |         |         |      A  |C        |         |         |         |         |
2.500D+00 |---------|---------|---------|---------|------A--|C--------|---------|---------|---------|---------|
2.750D+00 |         |         |         |         |      A  |C        |         |         |         |         |
3.000D+00 |         |         |         |         |      A  |C        |         |         |         |         |
3.250D+00 |         |         |         |         |      A  |C        |         |         |         |         |
3.500D+00 |         |         |         |         |      A  |C        |         |         |         |         |
3.750D+00 |---------|---------|---------|---------|------A--|CB-------|---------|---------|---------|---------|
4.000D+00 |         |         |         |         |       A |CB       |         |         |         |         |
4.250D+00 |         |         |         |         |       A | C       |         |         |         |         |
4.500D+00 |         |         |         |         |       A | C       |         |         |         |         |
4.750D+00 |         |         |         |         |       A | C       |         |         |         |         |
5.000D+00 |---------|---------|---------|---------|-------A-|-C-------|---------|---------|---------|---------|
5.250D+00 |         |         |         |         |       A | C       |         |         |         |         |
5.500D+00 |         |         |         |         |      A  | C       |         |         |         |         |
5.750D+00 |         |         |         |         |      A  |CB       |         |         |         |         |
6.000D+00 |         |         |         |         |     A   |CB       |         |         |         |         |
6.250D+00 |---------|---------|---------|---------|-----A---|CB-------|---------|---------|---------|---------|
6.500D+00 |         |         |         |         |     A   |CB       |         |         |         |         |
6.750D+00 |         |         |         |         |    A    |CB       |         |         |         |         |
7.000D+00 |         |         |         |         |    A    |CB       |         |         |         |         |
7.250D+00 |         |         |         |         |    A    |CB       |         |         |         |         |
7.500D+00 |---------|---------|---------|---------|----A----|CB-------|---------|---------|---------|---------|
7.750D+00 |         |         |         |         |    A    |CB       |         |         |         |         |
8.000D+00 |         |         |         |         |    A    |CB       |         |         |         |         |
8.250D+00 |         |         |         |         |    A    |CB       |         |         |         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 10
INDEPENDENT VARIABLE :TIMLOG      (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LH+          SCALE  1.0000D+01   A
LO2-         SCALE  1.0000D+01   B
LOH          SCALE  1.0000D+01   C
LOH-         SCALE  1.0000D+01   D
LHO2         SCALE  1.0000D+01   E
          0                                                0.5                                               1
1.146D-13 |---------|---------|---------|---------|----C----|--------E|---------|-------DB|-A-------|---------|
2.500D-01 |         |         |         |         |    C    |        E|         |       DB|  A      |         |
5.000D-01 |         |         |         |         |    C    |        E|         |       DB|  A      |         |
7.500D-01 |         |         |         |         |    C    |        E|         |       DB|  A      |         |
1.000D+00 |         |         |         |         |    C    |        E|         |       DB|  A      |         |
1.250D+00 |---------|---------|---------|---------|-----C---|--------E|---------|-------DB|-A-------|---------|
1.500D+00 |         |         |         |         |     C   |        E|         |       DB|  A      |         |
1.750D+00 |         |         |         |         |       C |        E|         |       DB|  A      |         |
2.000D+00 |         |         |         |         |         C        E|         |       DB|  A      |         |
2.250D+00 |         |         |         |         |         |C      E |         |       DB|  A      |         |
2.500D+00 |---------|---------|---------|---------|---------|-C-----E-|---------|-------DB|-A-------|---------|
2.750D+00 |         |         |         |         |         | C     E |         |       DB|  A      |         |
3.000D+00 |         |         |         |         |         |C      E |         |       DB|  A      |         |
3.250D+00 |         |         |         |         |         |C      E |         |       DB|  A      |         |
3.500D+00 |         |         |         |         |         |C      E |         |       DB|  A      |         |
3.750D+00 |---------|---------|---------|---------|---------|C------E-|---------|-------DB|-A-------|---------|
4.000D+00 |         |         |         |         |         C       E |         |       DB|  A      |         |
4.250D+00 |         |         |         |         |         C       E |         |       DB|  A      |         |
4.500D+00 |         |         |         |         |         C       E |         |       DB|  A      |         |
4.750D+00 |         |         |         |         |        C|       E |         |       DB|  A      |         |
5.000D+00 |---------|---------|---------|---------|--------C|-------E-|---------|-------BD|A--------|---------|
5.250D+00 |         |         |         |         |       C |      E  |         |       BD|A        |         |
5.500D+00 |         |         |         |         |       C |      E  |         |       BD|A        |         |
5.750D+00 |         |         |         |         |       C |      E  |         |      B D|A        |         |
6.000D+00 |         |         |         |         |       C |     E   |         |      B D|A        |         |
6.250D+00 |---------|---------|---------|---------|------C--|-----E---|---------|------B-D|A--------|---------|
6.500D+00 |         |         |         |         |     C   |    E    |         |     B  D|A        |         |
6.750D+00 |         |         |         |         |    C    |   E     |         |    B   D|A        |         |
7.000D+00 |         |         |         |         |  C      |  E      |         |   B    D|A        |         |
7.250D+00 |         |         |         |         |C        | E       |         |  B      D         |         |
7.500D+00 |---------|---------|---------|------C--|---------E---------|---------|-B-------D---------|---------|
7.750D+00 |         |         |         |  C      |       E |         |         B         D         |         |
8.000D+00 |         |         |         | C       |      E  |         |        B|         D         |         |
8.250D+00 |         |         |         |C        |      E  |         |        B|         D         |         |
```

```
PLOTTING PARAMETERS FOR GRAPH STREAM 11
INDEPENDENT VARIABLE :TIMLOG     (PLOTTED VERTICALLY)
DEPENDENT VARIABLES (PLOTTED HORIZONTALLY):
LE-          SCALE  1.0000D+01   A
LH           SCALE  1.0000D+01   B
LHO2-        SCALE  1.0000D+01   C
          0                                                0.5
1.146D-13 |---------|---------|---AB----|--------C|---------|---------|---------|---------|---------|---------|
2.500D-01 |         |         |   AB    |         |C        |         |         |         |         |         |
5.000D-01 |         |         |   AB    |         |   C     |         |         |         |         |         |
7.500D-01 |         |         |   AB    |         |     C   |         |         |         |         |         |
1.000D+00 |         |         |   AB    |         |        C|         |         |         |         |         |
1.250D+00 |---------|---------|---A-B---|---------|---------|C--------|---------|---------|---------|---------|
1.500D+00 |         |         |   A  B  |         |         |  C      |         |         |         |         |
1.750D+00 |         |         |    A B  |         |         |   C     |         |         |         |         |
2.000D+00 |         |         |    A B  |         |         |   C     |         |         |         |         |
2.250D+00 |         |         |     B   |         |         |  C      |         |         |         |         |
2.500D+00 |---------|---------|----BA---|---------|---------|-C-------|---------|---------|---------|---------|
2.750D+00 |         |         |    BA   |         |         | C       |         |         |         |         |
3.000D+00 |         |         |    BA   |         |         | C       |         |         |         |         |
3.250D+00 |         |         |    B    |         |         |  C      |         |         |         |         |
3.500D+00 |         |         |    B    |         |         |  C      |         |         |         |         |
3.750D+00 |---------|---------|---BA----|---------|---------|--C------|---------|---------|---------|---------|
4.000D+00 |         |         |   B     |         |         |   C     |         |         |         |         |
4.250D+00 |         |         |  BA     |         |         |   C     |         |         |         |         |
4.500D+00 |         |         |  BA     |         |         |   C     |         |         |         |         |
4.750D+00 |         |         |  B      |         |         |   C     |         |         |         |         |
5.000D+00 |---------|---------|--B------|---------|---------|---C-----|---------|---------|---------|---------|
5.250D+00 |         |         | B       |         |         |   C     |         |         |         |         |
5.500D+00 |         |         |BA       |         |         |   C     |         |         |         |         |
5.750D+00 |         |         BA        |         |         |   C     |         |         |         |         |
6.000D+00 |         |        B|A        |         |         |   C     |         |         |         |         |
6.250D+00 |---------|-------B-A---------|---------|---------|--C------|---------|---------|---------|---------|
6.500D+00 |         |     B A |         |         |         |  C      |         |         |         |         |
6.750D+00 |         |    B A  |         |         |         |   C     |         |         |         |         |
7.000D+00 |         |  B A    |         |         |         |   C     |         |         |         |         |
7.250D+00 |         |B A      |         |         |         |   C     |         |         |         |         |
7.500D+00 |------B-A|---------|---------|---------|---------|---C-----|---------|---------|---------|---------|
7.750D+00 |  B A    |         |         |         |         |   C     |         |         |         |         |
8.000D+00 |B  A     |         |         |         |         |   C     |         |         |         |         |
8.250D+00 |B A      |         |         |         |         |   C     |         |         |         |         |
```

APPENDIX K

IDENTIFICATION OF DOMINANT IONIC FORMS OF IMPURITY SPECIES

This appendix documents the results of equilibrium proportionation calculations used to assess the dominant ionic forms of impurities likely to be found in the post-accident coolant water at Millstone Unit I. The key results are summarized below.

Fe Impurities

With regard to Fe impurities:

- For the likely dissolved O_2 levels $[Fe^{+2}] \gg [Fe^{+3}]$ by many orders of magnitude throughout all pH ranges of interest.
- At lower water temperatures, where natural recombination is least thermodynamically favored, hydrolysis of Fe^{+2} ions is insufficient to yield appreciable concentrations of $Fe(OH)^{+}$ ions.
- At higher temperatures, where natural recombination is more thermodynamically favored, $Fe(OH)^{+}$ ions may be appreciable for mildly alkaline pH conditions.
- Assuming all iron impurities are in the +2 oxidation state is slightly conservative.

Cu Impurities

With regard to Cu impurities:

- The primary oxidation states are +1 and +2, while the +3 state is extremely rare.
- For Cu impurities in the anticipated ppb range, both Cu^{+} and Cu^{+2} are likely to be present in roughly equal amounts. Hence assumption that all Cu is in the +2 oxidation state for the reaction:

$$Cu^{+2} + OH \longrightarrow Cu^{+3} + OH^{-}$$

-is conservative.

- At lower temperatures where natural recombination is least favored thermodynamically, the impacts of hydrolysis in forming $Cu(OH)^+$ ions should be insignificant for the pH range of interest.
- Only at higher temperatures could hydrolyzed Copper ions be a significant consideration.
- By omission of the production of OH radicals via the reaction:

  $$Cu^+ + H_2O_2 \longrightarrow Cu^{+2} + OH + OH^- \quad k=2.3 \times 10^9$$

  the simple Jenks-Greiss criteria used to judge stability is grossly overconservative.

Mn Impurities

With regard to Mn impurities:

- Based on a review of the primary oxidation states of manganese, the +2 oxidation state is dominant while the +1 and +3 states are extremely rare.
- Hydrolyzed forms of Mn, e.g.: Mn(OH)+ are too rare to play any significant role on radiolysis/recommendation reactions.

K.1 Chemical Reactions Involving Fe Impurities

- Iron (Fe) is known to be a moderately good reducing agent based on the half cell reaction:

$$Fe^{+2} + 2e^- = Fe \qquad \mathcal{E}_o = -0.44\,V \qquad (K\text{-}1)$$

- The oxidation of Fe^{+2} to form Fe^{+3} is governed by the reaction:

$$Fe^{+3} + e^- = Fe^{+2} \qquad \mathcal{E}_o = 0.771\,V \qquad (K\text{-}2)$$

- By noting the following half cell reactions:

$$\begin{array}{ll} 2Fe^{+3} + 2e^- = 2Fe^{+2} & \mathcal{E}_o = 1.542\,V \\ \underline{H_2O = \tfrac{1}{2}O_2 + 2H^+ + 2e^-} & \underline{\mathcal{E}_o = -0.6145\,V} \\ 2Fe^{+3} + H_2O \rightleftharpoons 2Fe^{+2} + \tfrac{1}{2}O_2 + 2H^+ & \Delta\mathcal{E}_{NET} = .927\,V \end{array} \qquad (K\text{-}3)$$

it is evident that Fe^{+3} would naturally tend to convert back to Fe^{+2} except for the case where there is excess dissolved O_2 in the water. An equilibrium condition between Fe^{+2}/Fe^{+3} can be defined based on the Nernst equation:

$$\Delta\mathcal{E} = \Delta\mathcal{E}_{NET} - \frac{2.3\,RT}{n\,\mathcal{F}} \log_e \frac{[Fe^{+2}][O_2]^{1/4}[H^+]}{[Fe^{+3}]} \qquad (K\text{-}4)$$

$R = 1.98$ cal/°K

$\mathcal{F} = 23{,}061$ cal/V (Farraday's constant)

When equilibrium is reached $\Delta\mathcal{E} \cong 0$, then

$$Fe^{+3} + \tfrac{1}{2}H_2O \overset{K_{eq}}{\rightleftharpoons} Fe^{+2} + \tfrac{1}{4}O_2 + H^+ \qquad (\Delta\mathcal{E}_{NET} = .4635\,V)$$

$$0 = -.4635\,V - \frac{(2.3)(1.98)(298.15)}{(23,061)} \log_e \frac{[Fe^{+2}]_{eq}\,[O_2]_{eq}^{1/4}\,[H^+]_{eq}}{[Fe^{+3}]_{eq}} \qquad (K-5$$

-then:

$$K_{eq} = \frac{[Fe^{+2}]_{eq}\,[O_2]_{eq}^{1/4}\,[H^+]_{eq}}{[Fe^{+3}]_{eq}} = \exp\left\{\frac{-(.4635)(23061)}{(2.3)(1.98)(298.15)}\right\} = \overset{3.81167\times 1}{\text{[redacted]}} \qquad (K-6)$$

To derive a relationship dependent on $[O_2]_{eq}$ and pH:

$$\log_{10} K_{eq} = \log_{10} \frac{[Fe^{+2}]_{eq}}{[Fe^{+3}]_{eq}} + 1/4 \log_{10} [O_2]_{eq} + \log_{10} [H^+]_{eq} \qquad (K-7)$$

Solving for $[Fe^{+2}]_{eq} / [Fe^{+3}]_{eq}$ yields:

$$\log_{10} \frac{[Fe^{+2}]_{eq}}{[Fe^{+3}]_{eq}} = \log_{10} K_{eq} - 1/4 \log_{10} [O_2]_{eq} - \log_{10} [H^+]_{eq}$$

$$= \log_{10} K_{eq} - 1/4 \log_{10} [O_2]_{eq} + pH \qquad (K-8)$$

Thus:

$$\frac{[Fe^{+2}]_{eq}}{[Fe^{+3}]_{eq}} = K_{eq}\,[O_2]_{eq}^{-1/4}\,10^{pH} \qquad (K-9)$$

In Appendix F it was determined that: (at 25°C)

Min $[O_2]_{eq} = 4.64 \times 10^{-5}$ moles/liter

Max $[O_2]_{eq} = 5.15 \times 10^{-5}$ moles/liter

Using this data sensitivity calculations can be performed to examine Fe^{+2} / Fe^{+3} ratios.

pH	$\frac{[Fe^{+2}]_{eq}}{[Fe^{+3}]_{eq}}$ for Min $[O_2]_{eq}$	$\frac{[Fe^{+2}]_{eq}}{[Fe^{+3}]_{eq}}$ for Max $[O_2]_{eq}$
7.5	1.46×10^5	1.42×10^5
7.0	4.62×10^4	4.5×10^4
6.5	1.46×10^4	1.42×10^4
6.0	4.62×10^3	4.5×10^3
5.5	1.46×10^2	1.42×10^3

Based on these considerations Fe^{+2} is favored over Fe^{+3} ions.

- Another potential type of Fe impurities would be from hydrolysis of Fe^{+2} ions. This type reaction is summarized by:

$$Fe^{+2} + H_2O \rightleftharpoons Fe(OH)^+ + H^+ \qquad (K\text{-}10)$$

The equilibrium hydrolysis constant for this reaction wold be:

$$K_{eq} = \frac{[Fe^{+2}]_{eq}}{[Fe(OH)^+]_{eq}\,[H^+]_{eq}} \qquad (K\text{-}11)$$

Again the ratio of $Fe^{+2}/Fd(OH)^+$ ions can be obtained parametrica
for pH by:

$$\log_{10} K_{eq} = \log_{10} \frac{[Fe^{+2}]_{eq}}{[Fe(OH)^+]_{eq}\,[H^+]_{eq}} = \log_{10} \frac{[Fe^{+2}]_{eq}}{[Fe(OH)^+]_{eq}} - \log_{10} [H^+$$

$$= \log_{10} \frac{[Fe^{+2}]_{eq}}{[Fe(OH)^+]_{eq}} + pH \qquad (K\text{-}12)$$

Solving for the ratio yields:

$$\frac{[Fe^{+2}]_{eq}}{[Fe(OH)^{+}]_{eq}} = 10^{(\log_{10} K_{eq} - pH)} \qquad (K\text{-}13)$$

Reference 33 notes that $\log_{10} K_{eq} = +9.33$ at (25°C) and $\log_{10} K_{eq} = +7.41$ at 100°C. Using this data the following table was constructed

pH	$\frac{[Fe^{+2}]_{eq}}{[Fe(OH)^{+}]_{eq}}$ at 25°C	$\frac{[Fe^{+2}]_{eq}}{[Fe(OH)^{+}]_{eq}}$ at 100°C
7.5	67.61	0.813
7.0	2.14×10^{2}	2.57×10^{0}
6.5	6.76×10^{2}	8.13×10^{0}
6.0	2.14×10^{3}	2.57×10^{1}
5.5	6.76×10^{3}	8.13×10^{1}

Based on these calculations it is evident that Fe^{+2} should be predominant for the pH range of interest with $Fe(OH)^{+}$ only becoming important for higher temperatures, where recombination of H_2 is favored via

$$OH + H_2 \rightarrow H + (H_2O)$$

Having identified the predominate ionic species (e.g. mainly Fe^{+2}) the table on the following page summarizes the known reaction rates for radical species produced via radiolysis.

Impurity Reaction	Rate Constant	Reference
(1) $Fe^{+2} + OH \rightarrow Fe^{+3} + OH^-$	$k = 3.4 \times 10^8$	19
(2) $Fe^{+3} + H \rightarrow Fe^{+2} + H^+$	$k = 5.0 \times 10^8$	18
(3) $Fe^{+3} + e_{aq}^- \rightarrow Fe^{+2} + (H_2O)$	$k = 5.0 \times 10^{10}$	16
(4) $Fe^{+2} + HO_2 \rightarrow Fe^{+3} + HO_2^-$	$k = 2.1 \times 10^6$	19
(5) $Fe^{+3} + O_2^- \rightarrow Fe^{+2} + O_2$	$k = 1.55 \times 10^3$	19 *
(6) $Fe^{+3} + HO_2 \rightarrow Fe^{+2} + H^+ + O_2$	negligible	19

Based on this review reactions 1-5 should be considered.
— Reactions 1-3 will have the biggest impact.

Notes:

* Reference 19 notes that for $Fe^{+3} + O_2^- \rightarrow Fe^{+2} + O_2$,

$$k = \frac{3.6 \times 10^{-3}\ k(HO_2 + Fe^{+2})}{K_{eq}(HO_2)} \qquad (K\text{-}14)$$

-assuming $K_{eq}(HO_2)$, for reaction: $HO_2 \rightleftharpoons H^+ + O_2^-$ is 4.88 (Reference 19), then

$$k = \frac{(3.6 \times 10^{-3})(2.1 \times 10^6)}{4.88} = 1.55 \times 10^3 \qquad (K\text{-}15)$$

K.2 Chemical Reactions Involving Cu Impurities

- It must first be pointed out that treatment of Copper impurities is based on highly conservative assumptions of initial Cu impurities as compared to normal range.

- The primary oxidation states of Cu are +1, and +2. Reference 20 notes that the +3 oxidation state in Cu is extremely rare.

- Oxides of copper (Cu_2O) are extremely insoluble in water and can only be formed at high temperatures.

- From electrochemical considerations the Cu^+ ion is known to be unstable and tending to convert to Cu^{+2}

$$2\,Cu^+ = Cu + Cu^{+2} \qquad \Delta E_o = 0.18V \qquad \text{(K-16)}$$

[redacted]

-and:

$$K_{eq} = \frac{[Cu^{+2}]_{eq}}{[Cu^+]^2_{eq}} = 1.2\times10^6 \quad \text{at } T=25°C \qquad \text{(K-17}$$

-the relative ratio of concentrations can be obtained by noting:

$$[Cu^+]^2_{eq} = \frac{[Cu^{+2}]_{eq}}{K_{eq}} \Rightarrow [Cu^+]_{eq} = \sqrt{\frac{[Cu^{+2}]_{eq}}{K_{eq}}} \qquad \text{(K-18)}$$

Then:

$$\frac{[Cu^{+2}]_{eq}}{[Cu^+]_{eq}} = [Cu^{+2}]_{eq}^{1/2}\,K_{eq}^{1/2} \qquad \text{(K-19}$$

Assuming Cu impurities are in the range of 4.722×10^{-7} mol

then:

$$\frac{[Cu^{+2}]_{eq}}{[Cu^+]_{eq}} = (4.722\times10^{-7})^{1/2}(1.2\times10^6)^{1/2} = 0.753 \qquad \text{(K}$$

$[Cu^{+2}]_{eq}$	$\frac{[Cu^{+2}]_{eq}}{[Cu^{+}]_{eq}}$	
1×10^{-3}	34.64	
1×10^{-4}	10.95	
1×10^{-5}	3.46	
1×10^{-6}	1.095	
1×10^{-7}	0.346	
4.722×10^{-7}	0.753	← anticipated Cu ppb

Thus because of the "rare" Cu content Cu^{+}, Cu^{+2} will *both* be appreciable.

- Another potential forms of Cu impurities will be the hydrolyzed forms of Cu^{+2}, from the equilibrium reaction:

$$Cu^{+2} + H_2O \rightleftharpoons Cu(OH)^{+} + H^{+} \qquad \text{(K-21)}$$

The equilibrium hydrolysis constant for this reaction would be:

$$K_{eq} = \frac{[Cu^{+2}]_{eq}}{[Cu(OH)^{+}]_{eq}[H^{+}]_{eq}} \qquad \text{(K-22)}$$

The ratio of $Cu^{+}/Cu(OH)^{+}$ ions can be obtained parametrically for different pH values by:

$$\log_{10} K_{eq} = \log_{10} \frac{[Cu^{+2}]_{eq}}{[Cu(OH)^{+}]_{eq}} + pH \qquad \text{(K-23)}$$

The equilibrium ratio would be:

$$\frac{[Cu^{+2}]_{eq}}{[Cu(OH)^{+}]_{eq}} = 10^{(\log_{10} K_{eq} - pH)} \qquad (K\text{-}24)$$

The best estimate value of Keq (based on Reference 34) for T = 25°C is:

$$\log_{10} K_{eq} = 8.0 \qquad (K_{eq} = 1\times10^{8})$$

There is no good approximation or experimental value at 100°C in published literature. A reasonable extrapolation can be made based on the Law of Mass Action from chemical thermodynamics (Reference 35). Based on this law, Keq can be related to the Gibbs Free Energy function:

$$-RT \log_e K_{eq}(T) = \Delta G(T) \qquad (K\text{-}25)$$

Using the best estimate value of $K_{eq} = 1\times10^{8}$

$$\text{at } T=25°C: \ \Delta G(298.15) = -RT \log_e K_{eq}(298.15)$$

$$= -(1.98)(298.15) \log_e (1\times10^{8})$$

$$= -1.0874\times10^{4} \ \text{cal/mole} \qquad (K\text{-}26)$$

The extrapolated value of the Gibbs free energy is given by:

$$\Delta G(T_0+\Delta T) \cong \Delta G(T_0) - \Delta S(T_0)\Delta T + \int_{T_0}^{T_0+\Delta T} \overline{\Delta C_p}\, dT - (T_0+\Delta T)\int_{T_0}^{T_0+\Delta T} \frac{\overline{\Delta C_p}\, dT}{T}$$

(K-27)

Based on Reference 34: $\Delta S(T_0) = \Delta S(298.15) \cong 2.0$

$\overline{\Delta C_p} \cong -7.0$

Thus at $T = 100°C = 373.15°K$

$$\Delta G(373.15) \overset{\sim}{=}$$

$$= \Delta G(298.15) - \Delta S(298.15)(75°K) + \int_{298.15}^{373.15} \overline{\Delta C_p}\, dT - (373.15°K)\int_{298.15}^{373.15} \frac{\overline{\Delta C_p}\, dT}{T}$$

$$= -1.0874 \times 10^4 - (2.0)(75) + (-7.0)(75) - (373.15)(-7.0)\left[\log_e\left(\frac{373.15}{298.15}\right)\right]$$

$$= -1.0963 \times 10^4 \ \mathrm{cal/mole} \qquad \text{(K-28)}$$

Using this extrapolated value for $\Delta G(373.15)$:

$$K_{eq}(373.15) = \exp\left[-\frac{\Delta G(373.15)}{RT}\right]$$

$$= \exp\left[-\frac{-1.0963 \times 10^4}{(1.98)(373.15)}\right]$$

$$= 2.782 \times 10^6 \qquad \text{(K-29)}$$

For this value: $\log_{10} K_{eq} = 6.444$

The table on the following page summarizes the ratios for various temperatures:

pH	$\frac{[Cu^{+2}]_{eq}}{[Cu(OH)^{+}]_{eq}}$ at 25°C	$\frac{[Cu^{+2}]_{eq}}{[Cu(OH)^{+}]_{eq}}$ at 100°C
7.5	3.16×10^{0}	8.79×10^{-2}
7.0	1.0×10^{1}	2.78×10^{-1}
6.5	3.16×10^{1}	8.79×10^{-1}
6.0	1.0×10^{2}	2.78×10^{0}
5.5	3.16×10^{2}	8.79×10^{0}

Based on this review:

- Cu^{+}, Cu^{+2} and $Cu(OH)^{+}$ ions will be the more dominant forms of copper impurities present in the water.

- There is appreciable data for radical reactions with Cu^{+} and Cu^{+2} but data is lacking for radical reactions with $Cu(OH)^{+}$ other than reaction which produce:

$$Cu^{+2} + OH \longrightarrow \left\{ \begin{array}{l} Cu(OH)^{+2} \\ Cu(OH)_2^{+} \end{array} \right. \qquad k = 3.5 \times 10^{8}$$

- The reactions on the following page were determined to play a significant role in radiolysis/recombinations reactions.

	Impurity Reaction	Rate Constant	Reference
(1)	$Cu^{+2} + H \rightarrow Cu^{+} + H^{+}$	$k = 9.8 \times 10^{8}$	18
(2)	$Cu^{+2} + e_{aq}^{-} \rightarrow Cu^{+} + (H_2O)$	$k = 4.0 \times 10^{10}$	16
(3)	$Cu^{+} + HO_2 + (H_2O) \rightarrow Cu^{+2} + H_2O_2 + OH^{-}$	$k = 6.0 \times 10^{8}$	19
(4)	$Cu^{+} + H_2O_2 \rightarrow Cu^{+2} + OH + OH^{-}$	$k = 2.3 \times 10^{9}$	19
(5)	$Cu^{+2} + HO_2 \rightarrow Cu^{+} + H^{+} + O_2$	$k = 2.1 \times 10^{8}$	19*
(6)	$Cu^{+2} + OH \rightarrow Cu^{+3} + OH^{-}$	$k = 3.5 \times 10^{8}$	19
(7)	$Cu^{+3} + H \rightarrow Cu^{+2} + H^{+}$	$k = 9.8 \times 10^{8}$	†Assumption
(8)	$Cu^{+3} + e_{aq}^{-} \rightarrow Cu^{+2} + (H_2O)$	$k = 4.0 \times 10^{10}$	†Assumption

Notes:

* Reference 19 notes that for $Cu^{+2} + HO_2 \rightarrow Cu^{+} + H^{+} + O_2$

$$k = (1.03 \times 10^{2})\, k\, (Fe^{+2} + HO_2)$$

- Assuming $k(Fe^{+2} + HO_2) = 2.1 \times 10^{6}$, then:

$$k = (1.03 \times 10^{2})(2.1 \times 10^{6}) = 2.1 \times 10^{8}$$

† It is necessary to postulate a back reaction to preclude a net buildup of Cu^{+3} which is not a normal oxidation state of Cu. It is important to note that reaction (4) tends to procede faster than reaction (6). This is due to the fact that $[H_2O_2] >> [OH]$ (by several orders of magnitude and the reaction rate constant k is roughly a full order of magnitude than k_6. In that the

actual impact of Cu is to enhance natural recombination. The omission of this effect in the model amounts to a very substantial conservatism.

K.3 Chemical Reactions-Involving Mn Impurities

- Manganese (Mn) is a strong reducing agent as based on the half cell reaction:

$$Mn^{+2} + 2e^{-} = Mn \qquad \mathcal{E}_0 = -1.18V \qquad \text{(K-30)}$$

- The principle oxidation states of Mn are:

$$Mn^{+2},\ Mn^{+3},\ Mn^{+4},\ Mn^{+5},\ Mn^{+6},\ Mn^{+7}$$

- The dissolution of Mn in weakly acidic solution produces Mn^{+2}. In contrast to the +2 oxidation state of Titanium, Vanadium, and Chromium, Mn^{+2} has no reducing properties, and the reaction:

$$Mn^{+3} + e^{-} = Mn^{+2} \qquad \mathcal{E}_0 = 1.51V \qquad \text{(K-31)}$$

is indicative of the difficulty in oxidizing $Mn^{+2} \rightarrow Mn^{+3}$

- The normal reaction with OH radical proceeds mainly due redox potential of OH

$$\begin{array}{ll} Mn^{+2} = Mn^{+3} + e^{-} & \mathcal{E}_0 = -1.51V \\ OH + e^{-} = OH^{-} & \mathcal{E}_0 = 1.83V \\ \hline OH + Mn^{+2} = Mn^{+3} + OH^{-} & \Delta\mathcal{E}_{NET} = 0.32V \end{array} \qquad \text{(K-32)}$$

- The manganate ion, MnO_4^{-2} is not anticipated in the coolant water due to the fact its normal method of production involves boiling MnO_2 with strongly alkaline solutions.

- It is not possible to obtain significant concentrations of Mn^{+3} in aqueous solution due to the fact that Mn^{+3} is such a powerful oxidizing it is capable of evolving (or stripping) oxygen from water

$$\begin{array}{ll} Mn^{+3} + e^{-} = Mn^{+2} & \mathcal{E}_0 = 1.51V \\ Mn^{+3} + H_2O = MnO_2 + 4H^{+} + e^{-} & \mathcal{E}_0 = 0.95V \\ \hline 2Mn^{+3} + H_2O = Mn^{+2} + MnO_2 + 4H^{+} & \Delta\mathcal{E}_{NET} = 0.56V \end{array} \qquad \text{(K-33)}$$

This net reaction (K-33) highlights how Mn^{+3} is unstable with respect to disproportionation to Mn^{+2} and MnO_2. As a result of this there is essentially <u>no</u> solution chemistry of Mn^{+3}.

- Another potential type of Mn impurities would be from hydrolysis of Mn^{+2} ions. This type of reaction is summarized by:

$$Mn^{+2} + H_2O \rightleftharpoons Mn(OH)^{+} + H^{+} \qquad (K\text{-}34)$$

The equilibrium hydrolysis constant for this reaction would be:

$$K_{eq} = \frac{[Mn^{+2}]_{eq}}{[Mn(OH)^{+}]_{eq}\,[H^{+}]_{eq}} \qquad (K\text{-}35)$$

The ratio of $[Mn^{+2}]_{eq}/[Mn(OH)^{+}]_{eq}$ can be obtained parametrically for pH by:

$$\log_{10} K_{eq} = \log_{10} \frac{[Mn^{+2}]_{eq}}{[Mn(OH)^{+}]_{eq}\,[H^{+}]_{eq}}$$

$$= \log_{10} \frac{[Mn^{+2}]_{eq}}{[Mn(OH)^{+}]_{eq}} + pH \qquad (K\text{-}36)$$

Solving for the ratio yields:

$$\frac{[Mn^{+2}]_{eq}}{[Mn(OH)^{+}]_{eq}} = 10^{(\log_{10} K_{eq} - pH)} \qquad (K\text{-}37)$$

Reference 33 notes that:

$\log_{10} K_{eq} = 10.59$ at 25°C

$\log_{10} K_{eq} = 8.5$ at 100°C

Using this data, the following table was constructed

pH	$\frac{[Mn^{+2}]_{eq}}{[Mn(OH)^{+}]_{eq}}$ at 25°C	$\frac{[Mn^{+2}]_{eq}}{[Mn(OH)^{+}]_{eq}}$ at 100°C
7.5	1.23×10^{3}	1×10^{1}
7.0	3.89×10^{3}	3.16×10^{1}
6.5	1.23×10^{4}	1×10^{2}
6.0	3.89×10^{4}	3.16×10^{2}
5.5	1.23×10^{5}	1×10^{3}

From this analysis it can be concluded that hydrolysis Effects are essentially insignificant and the dominant ionic forms will be the +2 oxidation state.

The reactions in the following table were determined to play a significant role in radiolysis / recombination reactions

Impurity Reaction	Rate Constant	Reference
(1) $Mn^{+2} + e_{aq}^{-} \rightarrow Mn^{+} + (H_2O)$	k =	16
(2) $Mn^{+2} + OH \rightarrow Mn^{+3} + OH^{-}$	$k = 1.4 \times 10^{8}$	19
(3) $Mn^{+2} + H \rightarrow Mn^{+} + H^{+}$	$k = 3 \times 10^{7}$	18

Analysis of Post-Accident Combustible Gas
Control at Millstone Unit I

Volume III

Combustible Gas Solubility Data

TABLE 1; SOLUBILITY COEFFICIENT, MICROGRAM GAS PER GRAM OF LIQUID/ATM OR PPM OF GAS IN LIQUID/ATM 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
32	0.09	6.88E 01	3.00E 01	1.98E 00	1.72E 00	1.32E 03	4.06E 01
34	0.10	6.68E 01	2.90E 01	1.95E 00	1.70E 00	1.26E 03	3.89E 01
36	0,10	6.49E 01	2.81E 01	1.92E 00	1.69E 00	1.20E 03	3.74E 01
38	0.11	6.31E 01	2.72E 01	1.89E 00	1.67E 00	1.14E 03	3.61E 01
40	0.12	6.14E 01	2.64E 01	1.86E 00	1.66E 00	1.09E 03	3.48E 01
42	0.13	5.98E 01	2.57E 01	1.84E 00	1.64E 00	1.04E 03	3.36E 01
44	0.14	5.82E 01	2.50E 01	1.82E 00	1.63E 00	1.00E 03	3.24E 01
46	0.15	5.68E 01	2.43E 01	1.79E 00	1.62E 00	9.58E 02	3.14E 01
48	0.17	5.53E 01	2.37E 01	1.77E 00	1.60E 00	9.19E 02	3.04E 01
50	0.18	5.40E 01	2.31E 01	1.75E 00	1.59E 00	8.83E 02	2.95E 01
52	0.19	5.27E 01	2.25E 01	1.73E 00	1.58E 00	8.48E 02	2.86E 01
54	0.21	5.15E 01	2.20E 01	1.72E 00	1.57E 00	8.16E 02	2.78E 01
56	0.22	5.03E 01	2.15E 01	1.70E 00	1.56E 00	7.85E 02	2.70E 01
58	0.24	4.92E 01	2.10E 01	1.68E 00	1.56E 00	7.57E 02	2.63E 01
60	0.26	4.81E 01	2.06E 01	1.67E 00	1.55E 00	7.30E 02	2.56E 01
62	0.27	4.71E 01	2.02E 01	1.65E 00	1.54E 00	7.04E 02	2.50E 01
64	0.29	4.61E 01	1.98E 01	1.64E 00	1.53E 00	6.80E 02	2.44E 01
66	0.32	4.52E 01	1.94E 01	1.63E 00	1.53E 00	6.57E 02	2.38E 01
68	0.34	4.43E 01	1.90E 01	1.62E 00	1.52E 00	6.36E 02	2.33E 01
70	0.36	4.34E 01	1.87E 01	1.61E 00	1.51E 00	6.16E 02	2.27E 01
72	0.39	4.26E 01	1.84E 01	1.59E 00	1.51E 00	5.97E 02	2.22E 01
74	0.42	4.18E 01	1.81E 01	1.58E 00	1.50E 00	5.78E 02	2.18E 01
76	0.44	4.10E 01	1.78E 01	1.58E 00	1.50E 00	5.61E 02	2.13E 01
78	0.47	4.03E 01	1.75E 01	1.57E 00	1.50E 00	5.45E 02	2.09E 01
80	0.51	3.96E 01	1.72E 01	1.56E 00	1.49E 00	5.30E 02	2.05E 01
82	0.54	3.89E 01	1.70E 01	1.55E 00	1.49E 00	5.15E 02	2.01E 01
84	0.58	3.83E 01	1.67E 01	1.54E 00	1.49E 00	5.01E 02	1.98E 01
86	0.62	3.76E 01	1.65E 01	1.54E 00	1.49E 00	4.88E 02	1.94E 01
88	0.66	3.70E 01	1.63E 01	1.53E 00	1.49E 00	4.75E 02	1.91E 01
90	0.70	3.65E 01	1.61E 01	1.52E 00	1.49E 00	4.63E 02	1.88E 01
92	0.74	3.59E 01	1.59E 01	1.52E 00	1.49E 00	4.52E 02	1.85E 01
94	0.79	3.54E 01	1.57E 01	1.51E 00	1.49E 00	4.41E 02	1.82E 01
96	0.84	3.49E 01	1.55E 01	1.51E 00	1.49E 00	4.31E 02	1.79E 01
98	0.89	3.44E 01	1.53E 01	1.50E 00	1.49E 00	4.21E 02	1.76E 01
100	0.95	3.40E 01	1.52E 01	1.50E 00	1.49E 00	4.12E 02	1.74E 01
102	1.01	3.35E 01	1.50E 01	1.50E 00	1.49E 00	4.03E 02	1.72E 01
104	1.07	3.31E 01	1.49E 01	1.49E 00	1.49E 00	3.95E 02	1.69E 01
106	1.13	3.27E 01	1.47E 01	1.49E 00	1.49E 00	3.86E 02	1.67E 01
108	1.20	3.23E 01	1.46E 01	1.49E 00	1.50E 00	3.79E 02	1.65E 01
110	1.27	3.19E 01	1.45E 01	1.49E 00	1.50E 00	3.71E 02	1.63E 01
112	1.35	3.15E 01	1.43E 01	1.48E 00	1.50E 00	3.64E 02	1.61E 01
114	1.43	3.12E 01	1.42E 01	1.48E 00	1.51E 00	3.58E 02	1.59E 01
116	1.51	3.09E 01	1.41E 01	1.48E 00	1.51E 00	3.51E 02	1.57E 01
118	1.60	3.05E 01	1.40E 01	1.48E 00	1.52E 00	3.45E 02	1.56E 01

TABLE 1; SOLUBILITY COEFFICIENT, MICROGRAM GAS PER GRAM OF LIQUID/ATM OR PPM OF GAS IN LIQUID/ATM 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
120	1.69	3.02E 01	1.39E 01	1.48E 00	1.52E 00	3.39E 02	1.54E 01
122	1.79	2.99E 01	1.38E 01	1.48E 00	1.53E 00	3.34E 02	1.52E 01
124	1.89	2.96E 01	1.37E 01	1.48E 00	1.53E 00	3.28E 02	1.51E 01
126	2.00	2.94E 01	1.36E 01	1.48E 00	1.54E 00	3.23E 02	1.50E 01
128	2.11	2.91E 01	1.35E 01	1.48E 00	1.55E 00	3.18E 02	1.48E 01
130	2.22	2.89E 01	1.35E 01	1.48E 00	1.55E 00	3.14E 02	1.47E 01
132	2.34	2.86E 01	1.34E 01	1.48E 00	1.56E 00	3.09E 02	1.46E 01
134	2.47	2.84E 01	1.33E 01	1.48E 00	1.57E 00	3.05E 02	1.44E 01
136	2.60	2.82E 01	1.32E 01	1.49E 00	1.58E 00	3.01E 02	1.43E 01
138	2.74	2.80E 01	1.32E 01	1.49E 00	1.58E 00	2.97E 02	1.42E 01
140	2.89	2.78E 01	1.31E 01	1.49E 00	1.59E 00	2.93E 02	1.41E 01
142	3.04	2.76E 01	1.31E 01	1.49E 00	1.60E 00	2.90E 02	1.40E 01
144	3.20	2.74E 01	1.30E 01	1.49E 00	1.61E 00	2.86E 02	1.39E 01
146	3.37	2.72E 01	1.30E 01	1.50E 00	1.62E 00	2.83E 02	1.38E 01
148	3.54	2.71E 01	1.29E 01	1.50E 00	1.63E 00	2.80E 02	1.38E 01
150	3.72	2.69E 01	1.29E 01	1.50E 00	1.64E 00	2.77E 02	1.37E 01
152	3.91	2.68E 01	1.28E 01	1.51E 00	1.65E 00	2.74E 02	1.36E 01
154	4.10	2.66E 01	1.28E 01	1.51E 00	1.66E 00	2.71E 02	1.35E 01
156	4.31	2.65E 01	1.28E 01	1.51E 00	1.68E 00	2.69E 02	1.34E 01
158	4.52	2.64E 01	1.27E 01	1.52E 00	1.69E 00	2.66E 02	1.34E 01
160	4.74	2.62E 01	1.27E 01	1.52E 00	1.70E 00	2.64E 02	1.33E 01
162	4.97	2.61E 01	1.27E 01	1.52E 00	1.71E 00	2.61E 02	1.33E 01
164	5.21	2.60E 01	1.27E 01	1.53E 00	1.73E 00	2.59E 02	1.32E 01
166	5.46	2.59E 01	1.26E 01	1.53E 00	1.74E 00	2.57E 02	1.32E 01
168	5.72	2.58E 01	1.26E 01	1.54E 00	1.75E 00	2.55E 02	1.31E 01
170	5.99	2.58E 01	1.26E 01	1.54E 00	1.77E 00	2.53E 02	1.31E 01
172	6.27	2.57E 01	1.26E 01	1.55E 00	1.78E 00	2.52E 02	1.30E 01
174	6.57	2.56E 01	1.26E 01	1.55E 00	1.80E 00	2.50E 02	1.30E 01
176	6.87	2.55E 01	1.26E 01	1.56E 00	1.81E 00	2.48E 02	1.29E 01
178	7.18	2.55E 01	1.26E 01	1.57E 00	1.83E 00	2.47E 02	1.29E 01
180	7.51	2.54E 01	1.26E 01	1.57E 00	1.84E 00	2.45E 02	1.29E 01
182	7.85	2.54E 01	1.26E 01	1.58E 00	1.86E 00	2.44E 02	1.28E 01
184	8.20	2.53E 01	1.26E 01	1.59E 00	1.87E 00	2.43E 02	1.28E 01
186	8.57	2.53E 01	1.26E 01	1.59E 00	1.89E 00	2.41E 02	1.28E 01
188	8.95	2.52E 01	1.26E 01	1.60E 00	1.91E 00	2.40E 02	1.28E 01
190	9.34	2.52E 01	1.26E 01	1.61E 00	1.93E 00	2.39E 02	1.28E 01
192	9.75	2.52E 01	1.26E 01	1.61E 00	1.94E 00	2.38E 02	1.27E 01
194	10.17	2.52E 01	1.26E 01	1.62E 00	1.96E 00	2.37E 02	1.27E 01
196	10.61	2.52E 01	1.26E 01	1.63E 00	1.98E 00	2.36E 02	1.27E 01
198	11.06	2.52E 01	1.26E 01	1.63E 00	2.00E 00	2.36E 02	1.27E 01
200	11.53	2.51E 01	1.26E 01	1.64E 00	2.02E 00	2.35E 02	1.27E 01
202	12.01	2.51E 01	1.26E 01	1.65E 00	2.04E 00	2.34E 02	1.27E 01
204	12.51	2.52E 01	1.27E 01	1.66E 00	2.06E 00	2.33E 02	1.27E 01
206	13.03	2.52E 01	1.27E 01	1.67E 0C	2.08E 00	2.33E 02	1.27E 01
208	13.57	2.52F 01	1.27E 01	1.68E 00	2.10E 00	2.32E 02	1.27E 01

TABLE 1; SOLUBILITY COEFFICIENT, MICROGRAM GAS PER GRAM OF LIQUID/ATM OR PPM OF GAS IN LIQUID/ATM 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
210	14.12	2.52E 01	1.27E 01	1.68E 00	2.12E 00	2.32E 02	1.27E 01
212	14.70	2.52E 01	1.28E 01	1.69E 00	2.14E 00	2.31E 02	1.27E 01
214	15.29	2.52E 01	1.28E 01	1.70E 00	2.16E 00	2.31E 02	1.27E 01
216	15.90	2.53E 01	1.28E 01	1.71E 00	2.19E 00	2.31E 02	1.27E 01
218	16.53	2.53E 01	1.29E 01	1.72E 00	2.21E 00	2.30E 02	1.28E 01
220	17.19	2.53E 01	1.29E 01	1.73E 00	2.23E 00	2.30E 02	1.28E 01
222	17.86	2.54E 01	1.29E 01	1.74E 00	2.25E 00	2.30E 02	1.28E 01
224	18.56	2.54E 01	1.30E 01	1.75E 00	2.28E 00	2.30E 02	1.28E 01
226	19.27	2.55E 01	1.30E 01	1.76E 00	2.30E 00	2.30E 02	1.28E 01
228	20.01	2.55E 01	1.30E 01	1.77E 00	2.33E 00	2.30E 02	1.29E 01
230	20.78	2.56E 01	1.31E 01	1.78E 00	2.35E 00	2.30E 02	1.29E 01
232	21.57	2.57E 01	1.31E 01	1.79E 00	2.38E 00	2.30E 02	1.29E 01
234	22.38	2.57E 01	1.32E 01	1.80E 00	2.40E 00	2.30E 02	1.30E 01
236	23.22	2.58E 01	1.32E 01	1.81E 00	2.43E 00	2.30E 02	1.30E 01
238	24.06	2.59E 01	1.33E 01	1.83E 00	2.45E 00	2.30E 02	1.30E 01
240	24.97	2.60E 01	1.33E 01	1.84E 00	2.48E 00	2.30E 02	1.31E 01
242	25.86	2.61E 01	1.34E 01	1.85E 00	2.51E 00	2.30E 02	1.31E 01
244	26.83	2.61E 01	1.34E 01	1.86E 00	2.54E 00	2.31E 02	1.31E 01
246	27.80	2.62E 01	1.35E 01	1.87E 00	2.56E 00	2.31E 02	1.32E 01
248	28.80	2.63E 01	1.35E 01	1.88E 00	2.59E 00	2.31E 02	1.32E 01
250	29.82	2.64E 01	1.36E 01	1.90E 00	2.62E 00	2.32E 02	1.33E 01
252	30.88	2.65E 01	1.36E 01	1.91E 00	2.65E 00	2.32E 02	1.33E 01
254	31.97	2.67E 01	1.37E 01	1.92E 00	2.68E 00	2.33E 02	1.34E 01
256	33.09	2.68E 01	1.38E 01	1.94E 00	2.71E 00	2.33E 02	1.35E 01
258	34.24	2.69E 01	1.38E 01	1.95E 00	2.74E 00	2.34E 02	1.35E 01
260	35.43	2.70E 01	1.39E 01	1.96E 00	2.77E 00	2.34E 02	1.36E 01
262	36.64	2.71E 01	1.40E 01	1.98E 00	2.80E 00	2.35E 02	1.37E 01
264	37.89	2.73E 01	1.40E 01	1.99E 00	2.83E 00	2.35E 02	1.37E 01
266	39.18	2.74E 01	1.41E 01	2.00E 00	2.86E 00	2.36E 02	1.38E 01
268	40.50	2.75E 01	1.42E 01	2.02E 00	2.90E 00	2.37E 02	1.39E 01
270	41.86	2.77E 01	1.42E 01	2.03E 00	2.93E 00	2.38E 02	1.39E 01
272	43.25	2.78E 01	1.43E 01	2.05E 00	2.96E 00	2.38E 02	1.40E 01
274	44.68	2.80E 01	1.44E 01	2.06E 00	3.00E 00	2.39E 02	1.41E 01
276	46.15	2.81E 01	1.45E 01	2.08E 00	3.03E 00	2.40E 02	1.42E 01
278	47.65	2.83E 01	1.46E 01	2.09E 00	3.06E 00	2.41E 02	1.43E 01
280	49.20	2.84E 01	1.46E 01	2.11E 00	3.10E 00	2.42E 02	1.44E 01
282	50.79	2.86E 01	1.47E 01	2.12E 00	3.13E 00	2.43E 02	1.45E 01
284	52.41	2.88E 01	1.48E 01	2.14E 00	3.17E 00	2.44E 02	1.45E 01
286	54.08	2.89E 01	1.49E 01	2.15E 00	3.21E 00	2.45E 02	1.46E 01
288	55.79	2.91E 01	1.50E 01	2.17E 00	3.24E 00	2.46E 02	1.47E 01
290	57.55	2.93E 01	1.51E 01	2.19E 00	3.28E 00	2.47E 02	1.49E 01
292	59.35	2.95E 01	1.52E 01	2.20E 00	3.32E 00	2.48E 02	1.50E 01
294	61.19	2.97E 01	1.53E 01	2.22E 00	3.35E 00	2.49E 02	1.51E 01
296	63.08	2.99E 01	1.54E 01	2.24E 00	3.39E 00	2.50E 02	1.52E 01
298	65.02	3.01E 01	1.55E 01	2.25E 00	3.43E 00	2.51E 02	1.53E 01

TABLE 1; SOLUBILITY COEFFICIENT, MICROGRAM GAS PER GRAM OF LIQUID/ATM OR PPM OF GAS IN LIQUID/ATM 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
300	67.01	3.03E 01	1.56E 01	2.27E 00	3.47E 00	2.52E 02	1.54E 01
302	69.04	3.05E 01	1.57E 01	2.29E 00	3.51E 00	2.54E 02	1.56E 01
304	71.12	3.07E 01	1.58E 01	2.31E 00	3.55E 00	2.55E 02	1.57E 01
306	73.25	3.09E 01	1.59E 01	2.32E 00	3.59E 00	2.56E 02	1.58E 01
308	75.43	3.11E 01	1.60E 01	2.34E 00	3.63E 00	2.58E 02	1.60E 01
310	77.67	3.14E 01	1.61E 01	2.36E 00	3.67E 00	2.59E 02	1.61E 01
312	79.95	3.16E 01	1.62E 01	2.38E 00	3.71E 00	2.60E 02	1.63E 01
314	82.29	3.18E 01	1.63E 01	2.40E 00	3.75E 00	2.62E 02	1.64E 01
316	84.69	3.21E 01	1.64E 01	2.42E 00	3.80E 00	2.63E 02	1.66E 01
318	87.14	3.23E 01	1.65E 01	2.44E 00	3.84E 00	2.65E 02	1.67E 01
320	89.64	3.25E 01	1.67E 01	2.46E 00	3.88E 00	2.66E 02	1.69E 01
322	92.21	3.28E 01	1.68E 01	2.48E 00	3.93E 00	2.68E 02	1.71E 01
324	94.83	3.31E 01	1.39E 01	2.50E 00	3.97E 00	2.69E 02	1.72E 01
326	97.51	3.33E 01	1.70E 01	2.52E 00	4.02E 00	2.71E 02	1.74E 01
328	100.25	3.36E 01	1.72E 01	2.54E 00	4.06E 00	2.73E 02	1.76E 01
330	103.05	3.39E 01	1.73E 01	2.56E 00	4.11E 00	2.74E 02	1.78E 01
332	105.91	3.41E 01	1.74E 01	2.58E 00	4.15E 00	2.76E 02	1.80E 01
334	108.83	3.44E 01	1.76E 01	2.60E 00	4.20E 00	2.78E 02	1.82E 01
336	111.82	3.47E 01	1.77E 01	2.63E 00	4.25E 00	2.80E 02	1.84E 01
338	114.87	3.50E 01	1.78E 01	2.65E 00	4.29E 00	2.81E 02	1.87E 01
340	117.99	3.53E 01	1.80E 01	2.67E 00	4.34E 00	2.83E 02	1.89E 01
342	121.18	3.56E 01	1.81E 01	2.69E 00	4.39E 00	2.85E 02	1.91E 01
344	124.43	3.59E 01	1.83E 01	2.72E 00	4.44E 00	2.87E 02	1.94E 01
346	127.75	3.62E 01	1.84E 01	2.74E 00	4.49E 00	2.89E 02	1.96E 01
348	131.14	3.65E 01	1.86E 01	2.76E 00	4.54E 00	2.91E 02	1.99E 01
350	134.60	3.69E 01	1.87E 01	2.79E 00	4.59E 00	2.93E 02	2.02E 01
352	138.14	3.72E 01	1.89E 01	2.81E 00	4.64E 00	2.95E 02	2.05E 01
354	141.74	3.75E 01	1.90E 01	2.84E 00	4.69E 00	2.97E 02	2.08E 01
356	145.42	3.79E 01	1.92E 01	2.86E 00	4.74E 00	2.99E 02	2.11E 01
358	149.18	3.82E 01	1.94E 01	2.89E 00	4.80E 00	3.01E 02	2.14E 01
360	153.01	3.86E 01	1.95E 01	2.91E 00	4.85E 00	3.03E 02	2.17E 01
362	156.92	3.89E 01	1.97E 01	2.94E 00	4.90E 00	3.06E 02	2.21E 01
364	160.90	3.93E 01	1.99E 01	2.96E 00	4.96E 00	3.08E 02	2.24E 01
366	164.97	3.97E 01	2.00E 01	2.99E 00	5.01E 00	3.10E 02	2.28E 01
368	169.11	4.00E 01	2.02E 01	3.02E 00	5.06E 00	3.12E 02	2.32E 01
370	173.34	4.04E 01	2.04E 01	3.04E 00	5.12E 00	3.15E 02	2.36E 01
372	177.65	4.08E 01	2.06E 01	3.07E 00	5.18E 00	3.17E 02	2.41E 01
374	182.04	4.12E 01	2.08E 01	3.10E 00	5.23E 00	3.20E 02	2.45E 01
376	186.52	4.16E 01	2.09E 01	3.13E 00	5.29E 00	3.22E 02	2.50E 01
378	191.08	4.20E 01	2.11E 01	3.16E 00	5.34E 00	3.24E 02	2.55E 01
380	195.73	4.24E 01	2.13E 01	3.18E 00	5.40E 00	3.27E 02	2.60E 01
382	200.47	4.29E 01	2.15E 01	3.21E 00	5.46E 00	3.29E 02	2.66E 01
384	205.29	4.33E 01	2.17E 01	3.24E 00	5.52E 00	3.32E 02	2.72E 01
386	210.21	4.37E 01	2.19E 01	3.27E 00	5.58E 00	3.35E 02	2.78E 01
388	215.22	4.42E 01	2.21E 01	3.30E 00	5.64E 00	3.37E 02	2.85E 01

TABLE 1; SOLUBILITY COEFFICIENT, MICROGRAM GAS PER GRAM OF LIQUID/ATM OR PPM OF GAS IN LIQUID/ATM 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
390	220.32	4.46E 01	2.24E 01	3.33E 00	5.70E 00	3.40E 02	2.92E 01
392	225.52	4.51E 01	2.26E 01	3.36E 00	5.76E 00	3.43E 02	3.00E 01
394	230.81	4.55E 01	2.28E 01	3.40E 00	5.82E 00	3.46E 02	3.08E 01
396	236.19	4.60E 01	2.30E 01	3.43E 00	5.88E 00	3.48E 02	3.17E 01
398	241.66	4.65E 01	2.32E 01	3.46E 00	5.94E 00	3.51E 02	3.27E 01
400	247.26	4.70E 01	2.35E 01	3.49E 00	6.01E 00	3.54E 02	3.38E 01
402	252.94	4.74E 01	2.37E 01	3.52E 00	6.07E 00	3.57E 02	3.50E 01
404	258.73	4.79E 01	2.39E 01	3.56E 00	6.13E 00	3.60E 02	3.63E 01
406	264.61	4.84E 01	2.42E 01	3.59E 00	6.20E 00	3.63E 02	3.78E 01
408	270.60	4.90E 01	2.44E 01	3.62E 00	6.26E 00	3.66E 02	3.96E 01
410	276.69	4.95E 01	2.47E 01	3.66E 00	6.33E 00	3.69E 02	4.16E 01
412	282.89	5.00E 01	2.49E 01	3.69E 00	6.39E 00	3.72E 02	4.43E 01
414	289.20	5.06E 01	2.52E 01	3.73E 00	6.46E 00	3.75E 02	4.78E 01
416	295.62	5.11E 01	2.54E 01	3.77E 00	6.52E 00	3.78E 02	5.42E 01
418	302.14	5.17E 01	2.57E 01	3.80E 00	6.59E 00	3.82E 02	
420	308.78	5.22E 01	2.60E 01	3.84E 00	6.66E 00	3.85E 02	
422	315.53	5.28E 01	2.62E 01	3.88E 00	6.73E 00	3.88E 02	
424	322.39	5.34E 01	2.65E 01	3.91E 00	6.80E 00	3.92E 02	
426	329.37	5.40E 01	2.68E 01	3.95E 00	6.87E 00	3.95E 02	
428	336.46	5.46E 01	2.71E 01	3.99E 00	6.94E 00	3.98E 02	
430	343.67	5.52E 01	2.74E 01	4.03E 00	7.01E 00	4.02E 02	
432	351.00	5.58E 01	2.77E 01	4.07E 00	7.08E 00	4.05E 02	
434	358.46	5.64E 01	2.80E 01	4.11E 00	7.15E 00	4.09E 02	
436	366.03	5.70E 01	2.83E 01	4.15E 00	7.22E 00	4.13E 02	
438	373.72	5.77E 01	2.86E 01	4.19E 00	7.29E 00	4.16E 02	
440	381.54	5.83E 01	2.89E 01	4.23E 00	7.37E 00	4.20E 02	
442	389.42	5.90E 01	2.93E 01	4.27E 00	7.44E 00	4.24E 02	
444	397.56	5.97E 01	2.96E 01	4.32E 00	7.51E 00	4.27E 02	
446	405.76	6.03E 01	2.99E 01	4.36E 00	7.59E 00	4.31E 02	
448	414.09	6.10E 01	3.03E 01	4.40E 00	7.66E 00	4.35E 02	
450	422.55	6.17E 01	3.06E 01	4.45E 00	7.74E 00	4.39E 02	
452	431.14	6.24E 01	3.10E 01	4.49E 00	7.81E 00	4.43E 02	
454	439.87	6.32E 01	3.13E 01	4.54E 00	7.89E 00	4.47E 02	
456	448.73	6.39E 01	3.17E 01	4.58E 00	7.97E 00	4.51E 02	
458	457.73	6.46E 01	3.21E 01	4.63E 00	8.05E 00	4.55E 02	
460	466.87	6.54E 01	3.25E 01	4.68E 00	8.12E 00	4.59E 02	
462	476.14	6.62E 01	3.28E 01	4.73E 00	8.20E 00	4.63E 02	
464	485.56	6.69E 01	3.32E 01	4.77E 00	8.28E 00	4.68E 02	
466	495.12	6.77E 01	3.36E 01	4.82E 00	8.36E 00	4.72E 02	
468	504.83	6.85E 01	3.40E 01	4.87E 00	8.44E 00	4.76E 02	
470	514.37	6.93E 01	3.45E 01	4.92E 00	8.52E 00	4.81E 02	
472	524.67	7.02E 01	3.49E 01	4.97E 00	8.61E 00	4.85E 02	
474	534.81	7.10E 01	3.53E 01	5.03E 00	8.69E 00	4.89E 02	
476	545.11	7.18E 01	3.58E 01	5.08E 00	8.77E 00	4.94E 02	
478	555.55	7.27E 01	3.62E 01	5.13E 00	8.85E 00	4.99E 02	

TABLE 1; SOLUBILITY COEFFICIENT, MICROGRAM GAS PER GRAM OF LIQUID/ATM OR PPM OF GAS IN LIQUID/ATM 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
480	566.15	7.36E 01	3.67E 01	5.18E 00	8.94E 00	5.03E 02	
482	576.90	7.45E 01	3.71E 01	5.24E 00	9.02E 00	5.08E 02	
484	587.81	7.53E 01	3.76E 01	5.29E 00	9.11E 00	5.13E 02	
486	598.87	7.63E 01	3.81E 01	5.35E 00	9.19E 00	5.17E 02	
488	610.10	7.72E 01	3.86E 01	5.41E 00	9.28E 00	5.22E 02	
490	621.48	7.81E 01	3.91E 01	5.46E 00	9.36E 00	5.27E 02	
492	633.03	7.91E 01	3.96E 01	5.52E 00	9.45E 00	5.32E 02	
494	644.73	8.00E 01	4.01E 01	5.58E 00	9.54E 00	5.37E 02	
496	656.61	8.10E 01	4.07E 01	5.64E 00	9.63E 00	5.42E 02	
498	668.65	8.20E 01	4.12E 01	5.70E 00	9.71E 00	5.47E 02	
500	680.86	8.30E 01	4.18E 01	5.76E 00	9.80E 00	5.52E 02	
502	693.23	8.40E 01	4.24E 01	5.83E 00	9.89E 00	5.57E 02	
504	705.78	8.51E 01	4.29E 01	5.89E 00	9.98E 00	5.63E 02	
506	718.50	8.61E 01	4.35E 01	5.95E 00	1.01E 01	5.68E 02	
508	731.40	8.72E 01	4.41E 01	6.02E 00	1.02E 01	5.73E 02	
510	744.47	8.82E 01	4.48E 01	6.08E 00	1.03E 01	5.79E 02	
512	757.72	8.93E 01	4.54E 01	6.15E 00	1.04E 01	5.84E 02	
514	771.15	9.04E 01	4.60E 01	6.22E 00	1.04E 01	5.90E 02	
516	784.76	9.16E 01	4.67E 01	6.29E 00	1.05E 01	5.95E 02	
518	798.55	9.27E 01	4.74E 01	6.36E 00	1.06E 01	6.01E 02	
520	812.53	9.39E 01	4.81E 01	6.43E 00	1.07E 01	6.07E 02	
522	826.69	9.50E 01	4.88E 01	6.50E 00	1.08E 01	6.12E 02	
524	841.04	9.62E 01	4.95E 01	6.57E 00	1.09E 01	6.18E 02	
526	855.58	9.74E 01	5.02E 01	6.64E 00	1.10E 01	6.24E 02	
528	870.31	9.87E 01	5.10E 01	6.72E 00	1.11E 01	6.30E 02	
530	885.23	9.99E 01	5.18E 01	6.79E 00	1.12E 01	6.36E 02	
532	900.34	1.01E 02	5.25E 01	6.87E 00	1.13E 01	6.42E 02	
534	915.66	1.02E 02	5.34E 01	6.95E 00	1.14E 01	6.48E 02	
536	931.17	1.04E 02	5.42E 01	7.03E 00	1.15E 01	6.55E 02	
538	946.88	1.05E 02	5.50E 01	7.11E 00	1.16E 01	6.61E 02	
540	962.79	1.06E 02	5.59E 01	7.19E 00	1.17E 01	6.67E 02	
542	978.90	1.08E 02	5.68E 01	7.27E 00	1.18E 01	6.74E 02	
544	995.22	1.09E 02	5.77E 01	7.35E 00	1.19E 01	6.80E 02	
546	1011.75	1.10E 02	5.87E 01	7.44E 00	1.20E 01	6.87E 02	
548	1028.49	1.12E 02	5.96E 01	7.53E 00	1.21E 01	6.93E 02	
550	1045.43	1.13E 02	6.06E 01	7.61E 00	1.22E 01	7.00E 02	
552	1062.59	1.15E 02	6.16E 01	7.70E 00	1.23E 01	7.06E 02	
554	1079.96	1.16E 02	6.27E 01	7.79E 00	1.24E 01	7.13E 02	
556	1097.55	1.18E 02	6.37E 01	7.88E 00	1.25E 01	7.20E 02	
558	1115.36	1.19E 02	6.48E 01	7.98E 00	1.26E 01	7.27E 02	
560	1133.38	1.21E 02	6.60E 01	8.07E 00	1.27E 01	7.34E 02	
562	1151.63	1.22E 02	6.71E 01	8.17E 00	1.28E 01	7.41E 02	
564	1170.10	1.24E 02	6.83E 01	8.27E 00	1.30E 01	7.48E 02	
566	1188.80	1.25E 02	6.96E 01	8.36E 00	1.31E 01	7.55E 02	
568	1207.72	1.27E 02	7.08E 01	8.46E 00	1.32E 01	7.63E 02	

TABLE 1; SOLUBILITY COEFFICIENT, MICROGRAM GAS PER GRAM OF LIQUID/ATM OR PPM OF GAS IN LIQUID/ATM 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
570	1226.88	1.29E 02	7.21E 01	8.57E 00	1.33E 01	7.70E 02	
572	1246.26	1.30E 02	7.35E 01	8.67E 00	1.34E 01	7.77E 02	
574	1265.89	1.32E 02	7.49E 01	8.78E 00	1.35E 01	7.85E 02	
576	1285.74	1.34E 02	7.63E 01	8.88E 00	1.36E 01	7.92E 02	
578	1305.84	1.36E 02	7.78E 01	8.99E 00	1.37E 01	8.00E 02	
580	1326.17	1.37E 02	7.93E 01	9.10E 00	1.38E 01	8.08E 02	
582	1346.75	1.39E 02	8.09E 01	9.21E 00	1.39E 01	8.15E 02	
584	1367.57	1.41E 02	8.25E 01	9.33E 00	1.41E 01	8.23E 02	
586	1388.54	1.43E 02	8.42E 01	9.45E 00	1.42E 01	8.31E 02	
588	1409.96	1.45E 02	8.60E 01	9.56E 00	1.43E 01	8.39E 02	
590	1431.52	1.46E 02	8.78E 01	9.68E 00	1.44E 01	8.47E 02	
592	1453.35	1.48E 02	8.97E 01	9.81E 00	1.45E 01	8.55E 02	
594	1475.42	1.50E 02	9.16E 01	9.93E 00	1.46E 01	8.64E 03	
596	1497.76	1.52E 02	9.37E 01	1.01E 01	1.47E 01	8.72E 02	
598	1520.36	1.54E 02	9.58E 01	1.02E 01	1.49E 01	8.80E 02	
600	1543.22	1.56E 02	9.80E 01	1.03E 01	1.50E 01	8.89E 02	

TABLE 2; MASS CONCENTRATION RATIO, MICROGRAM PER GRAM GAS/MICROGRAM PER GRAM LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
32	0.09	4.28E 06	8.60E 06	9.39E 06	2.14E 07	9.16E 05	3.64E 06
34	0.10	4.07E 06	8.21E 06	8.80E 06	2.00E 07	8.88E 05	3.50E 06
36	0.10	3.87E 06	7.82E 06	8.25E 06	1.86E 07	8.60E 05	3.36E 06
38	0.11	3.67E 06	7.46E 06	7.73E 06	1.74E 07	8.32E 05	3.22E 06
40	0.12	3.49E 06	7.10E 06	7.25E 06	1.62E 07	8.06E 05	3.09E 06
42	0.13	3.32E 06	6.77E 06	6.80E 06	1.51E 07	7.79E 05	2.97E 06
44	0.14	3.16E 06	6.44E 06	6.38E 06	1.41E 07	7.54E 05	2.84E 06
46	0.15	3.00E 06	6.13E 06	5.98E 06	1.32E 07	7.29E 05	2.72E 06
48	0.17	2.85E 06	5.84E 06	5.61E 06	1.23E 07	7.05E 05	2.60E 06
50	0.18	2.71E 06	5.56E 06	5.27E 06	1.15E 07	6.81E 05	2.49E 06
52	0.19	2.58E 06	5.29E 06	4.94E 06	1.08E 07	6.58E 05	2.38E 06
54	0.21	2.46E 06	5.03E 06	4.64E 06	1.01E 07	6.36E 05	2.28E 06
56	0.22	2.34E 06	4.78E 06	4.36E 06	9.40E 06	6.14E 05	2.18E 06
58	0.24	2.22E 06	4.55E 06	4.09E 06	8.80E 06	5.93E 05	2.08E 06
60	0.26	2.12E 06	4.33E 06	3.84E 06	8.23E 06	5.73E 05	1.99E 06
62	0.27	2.01E 06	4.11E 06	3.61E 06	7.71E 06	5.53E 05	1.90E 06
64	0.29	1.92E 06	3.91E 06	3.39E 06	7.21E 06	5.33E 05	1.82E 06
66	0,32	1.83E 06	3.72E 06	3.18E 06	6.76E 06	5.14E 05	1.74E 06
68	0.34	1.74E 06	3.54E 06	3.00E 06	6.33E 06	4.96E 05	1.66E 06
70	0.36	1.66E 06	3.36E 06	2.82E 06	5.93E 06	4.79E 05	1.58E 06
72	0.39	1.58E 06	3.20E 06	2.65E 06	5.56E 06	4.62E 05	1.51E 06
74	0.42	1.50E 06	3.04E 06	2.49E 06	5.21E 06	4.45E 05	1.44E 06
76	0.44	1.43E 06	2.89E 06	2.35E 06	4.89E 06	4.29E 05	1.38E 06
78	0.47	1.36E 06	2.75E 06	2.21E 06	4.59E 06	4.13E 05	1.32E 06
80	0.51	1.30E 06	2.61E 06	2.08E 06	4.30E 06	3.98E 05	1.26E 06
82	0.54	1.24E 06	2.48E 06	1.96E 06	4.04E 06	3.84E 05	1.20E 06
84	0.58	1.18E 06	2.36E 06	1.84E 06	3.79E 06	3.70E 05	1.15E 06
86	0.62	1.13E 06	2.25E 06	1.74E 06	3.56E 06	3.56E 05	1.09E 06
88	0.66	1.07E 06	2.14E 06	1.64E 06	3.34E 06	3.43E 05	1.04E 06
90	0.70	1.02E 06	2.03E 06	1.54E 06	3.14E 06	3.30E 05	9.97E 05
92	0.74	9.75E 05	1.93E 06	1.45E 06	2.95E 06	3.18E 05	9.51E 05
94	0.79	9.30E 05	1.84E 06	1.37E 06	2.77E 06	3.06E 05	9.08E 05
96	0.84	8.87E 05	1.75E 06	1.29E 06	2.61E 06	2.95E 05	8.67E 05
98	0.89	8.47E 05	1.66E 06	1.22E 06	2.45E 06	2.84E 05	8.28E 05
100	0.95	8.08E 05	1.58E 06	1.15E 06	2.31E 06	2.73E 05	7.91E 05
102	1.01	7.71E 05	1.51E 06	1.09E 06	2.17E 06	2.63E 05	7.55E 05
104	1.07	7.36E 05	1.43E 06	1.03E 06	2.04E 06	2.53E 05	7.21E 05
106	1.13	7.02E 05	1.36E 06	9.69E 05	1.92E 06	2.44E 05	6.89E 05
108	1.20	6.70E 05	1.30E 06	9.15E 05	1.81E 06	2.34E 05	6.58E 05
110	1.27	6.40E 05	1.24E 06	8.65E 05	1.70E 06	2.25E 05	6.28E 05
112	1.35	6.11E 05	1.18E 06	8.17E 05	1.60E 06	2.17E 05	6.00E 05
114	1.43	5.83E 05	1.12E 06	7.73E 05	1.51E 06	2.09E 05	5.73E 05
116	1.51	5.57E 05	1.07E 06	7.30E 05	1.42E 06	2.01E 05	5.48E 05
118	1.60	5.32E 05	1.02E 06	6.91E 05	1.34E 06	1.93E 05	5.23E 05

TABLE 2; MASS CONCENTRATION RATIO, MICROGRAM PER GRAM GAS/MICROGRAM PER GRAM LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
120	1.69	5.08E 05	9.68E 05	6.54E 05	1.26E 06	1.86E 05	5.00E 05
122	1.79	4.86E 05	9.22E 05	6.18E 05	1.19E 06	1.79E 05	4.78E 05
124	1.89	4.64E 05	8.78E 05	5.85E 05	1.12E 06	1.72E 05	4.57E 05
126	2.00	4.43E 05	8.37E 05	5.54E 05	1.06E 06	1.65E 05	4.36E 05
128	2.11	4,24E 05	7.98E 05	5.25E 05	9.98E 05	1.59E 05	4.17E 05
130	2.22	4.05E 05	7.60E 05	4.97E 05	9.41E 05	1.53E 05	3.99E 05
132	2.34	3.87E 05	7.25E 05	4.71E 05	8.88E 05	1.47E 05	3.81E 05
134	2.47	3.70E 05	6.91E 05	4.46E 05	8.38E 05	1.41E 05	3.65E 05
136	2.60	3.54E 05	6.59E 05	4.23E 05	7.91E 05	1.36E 05	3.49E 05
138	2.74	3.38E 05	6.28E 05	4.01E 05	7.47E 05	1.31E 05	3.34E 05
140	2.89	3.23E 05	5.99E 05	3.80E 05	7.06E 05	1.26E 05	3.19E 05
142	3.04	3.09E 05	5.72E 05	3.61E 05	6.66E 05	1.21E 05	3.05E 05
144	3.20	2.96E 05	5.45E 05	3.42E 05	6.30E 05	1.16E 05	2.92E 05
146	3.37	2.83E 05	5.20E 05	3.25E 05	5.95E 05	1.12E 05	2.79E 05
148	3.54	2.71E 05	4.97E 05	3.08E 05	5.62E 05	1.08E 05	2.67E 05
150	3.72	2.59E 05	4.74E 05	2.92E 05	5.31E 05	1.03E 05	2.56E 05
152	3.91	2.48E 05	4.52E 05	2.78E 05	5.02E 05	9.94E 04	2.45E 05
154	4.10	2.37E 05	4.32E 05	2.64E 05	4.75E 05	9.56E 04	2.34E 05
156	4.31	2.27E 05	4.12E 05	2.51E 05	4.49E 05	9.19E 04	2.24E 05
158	4.52	2.17E 05	3.94E 05	2.38E 05	4.25E 05	8.84E 04	2.15E 05
160	4.74	2.08E 05	3.76E 05	2.26E 05	4.02E 05	8.50E 04	2.06E 05
162	4.97	1.99E 05	3.59E 05	2.15E 05	3.81E 05	8.17E 04	1.97E 05
164	5.21	1.91E 05	3.43E 05	2.05E 05	3.60E 05	7.86E 04	1.89E 05
166	5.46	1.83E 05	3.28E 05	1.95E 05	3.41E 05	7.56E 04	1.81E 05
168	5.72	1.75E 05	3.14E 05	1.85E 05	3.23E 05	7.27E 04	1.73E 05
170	5.99	1.68E 05	3.00E 05	1.76E 05	3.06E 05	6.99E 04	1.66E 05
172	6.27	1.61E 05	2.87E 05	1.68E 05	2.90E 05	6.72E 04	1.59E 05
174	6.57	1.54E 05	2.74E 05	1.60E 05	2.74E 05	6.47E 04	1.52E 05
176	6.87	1.47E 05	2.62E 05	1.52E 05	2.60E 05	6.22E 04	1.46E 05
178	7.18	1.41E 05	2.51E 05	1.45E 05	2.46E 05	5.98E 04	1.40E 05
180	7.51	1.35E 05	2.40E 05	1.38E 05	2.34E 05	5.75E 04	1.34E 05
182	7.85	1.30E 05	2.29E 05	1.31E 05	2.22E 05	5.53E 04	1.28E 05
184	8.20	1.24E 05	2.19E 05	1.25E 05	2.10E 05	5.32E 04	1.23E 05
186	8.57	1.19E 05	2.10E 05	1.19E 05	1.99E 05	5.12E 04	1.18E 05
188	8.95	1.14E 05	2.01E 05	1.14E 05	1.89E 05	4.92E 04	1.13E 05
190	9.34	1.10E 05	1.92E 05	1.08E 05	1.79E 05	4.74E 04	1.09E 05
192	9.75	1.05E 05	1.84E 05	1.03E 05	1.70E 05	4.56E 04	1.04E 05
194	10.17	1.01E 05	1.76E 05	9.86E 04	1.62E 05	4.38E 04	9.99E 04
196	10.61	9.66E 04	1.69E 05	9.40E 04	1.53E 05	4.22E 04	9.58E 04
198	11.06	9.26E 04	1.62E 05	8.97E 04	1.46E 05	4.06E 04	9.13E 04
200	11.53	8.88E 04	1.55E 05	8.57E 04	1.38E 05	3.90E 04	8.82E 04
202	12.01	8.52E 04	1.48E 05	8.18E 04	1.32E 05	3.76E 04	8.46E 04
204	12.51	8.18E 04	1.42E 05	7.81E 04	1.25E 05	3.61E 04	8.12E 04
206	13.03	7.84E 04	1.36E 05	7.46E 04	1.19E 05	3.48E 04	7.79E 04
208	13.57	7.53E 04	1.30E 05	7.12E 04	1.13E 05	3.35E 04	7.48E 04

TABLE 21 MASS CONCENTRATION RATIO, MICROGRAM PER GRAM GAS/MICROGRAM PER GRAM LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
210	14.12	7.22E 04	1.25E 05	6.80E 04	1.07E 05	3.22E 04	7.18E 04
212	14.70	6.93E 04	1.20E 05	6.50E 04	1.02E 05	3.10E 04	6.89E 04
214	15.29	6.65E 04	1.15E 05	6.21E 04	9.71E 04	2.98E 04	6.62E 04
216	15.90	6.39E 04	1.10E 05	5.94E 04	9.24E 04	2.87E 04	6.35E 04
218	16.53	6.13E 04	1.06E 05	5.68E 04	8.79E 04	2.76E 04	6.10E 04
220	17.19	5.89E 04	1.01E 05	5.43E 04	8.36E 04	2.66E 04	5.86E 04
222	17.86	5.65E 04	9.72E 04	5.19E 04	7.96E 04	2.56E 04	5.62E 04
224	18.56	5.43E 04	9.33E 04	4.97E 04	7.58E 04	2.46E 04	5.40E 04
226	19.27	5.21E 04	8.95E 04	4.75E 04	7.22E 04	2.37E 04	5.19E 04
228	20.01	5.00E 04	8.59E 04	4.55E 04	6.87E 04	2.28E 04	4.98E 04
230	20.78	4.81E 04	8.24E 04	4.35E 04	6.55E 04	2.20E 04	4.79E 04
232	21.57	4.62E 04	7.91E 04	4.17E 04	6.24E 04	2.12E 04	4.60E 04
234	22.38	4.44E 04	7.59E 04	3.99E 04	5.95E 04	2.04E 04	4.42E 04
236	23.22	4.26E 04	7.29E 04	3.82E 04	5.67E 04	1.96E 04	4.25E 04
238	24.08	4.09E 04	7.00E 04	3.66E 04	5.40E 04	1.89E 04	4.08E 04
240	24.97	3.93E 04	6.72E 04	3.50E 04	5.15E 04	1.82E 04	3.92E 04
242	25.88	3.78E 04	6.46E 04	3.36E 04	4.91E 04	1.75E 04	3.77E 04
244	26.83	3.63E 04	6.20E 04	3.22E 04	4.69E 04	1.69E 04	3.62E 04
246	27.80	3.49E 04	5.96E 04	3.08E 04	4.47E 04	1.63E 04	3.48E 04
248	28.80	3.36E 04	5.72E 04	2.95E 04	4.27E 04	1.57E 04	3.35E 04
250	29.82	3.23E 04	5.50E 04	2.83E 04	4.07E 04	1.51E 04	3.22E 04
252	30.88	3.10E 04	5.29E 04	2.72E 04	3.89E 04	1.45E 04	3.09E 04
254	31.97	2.98E 04	5.08E 04	2.60E 04	3.71E 04	1.40E 04	2.97E 04
256	33.09	2.87E 04	4.88E 04	2.50E 04	3.54E 04	1.35E 04	2.86E 04
258	34.24	2.76E 04	4.69E 04	2.40E 04	3.38E 04	1.30E 04	2.75E 04
260	35.43	2.65E 04	4.51E 04	2.30E 04	3.23E 04	1.25E 04	2.64E 04
262	36.64	2.55E 04	4.34E 04	2.21E 04	3.09E 04	1.21E 04	2.54E 04
264	37.89	2.45E 04	4.17E 04	2.12E 04	2.95E 04	1.16E 04	2.44E 04
266	39.18	2.06E 04	4.01E 04	2.03E 04	2.82E 04	1.12E 04	2.35E 04
268	40.50	2.27E 04	3.86E 04	1.95E 04	2.70E 04	1.08E 04	2.26E 04
270	41.86	2.18E 04	3.71E 04	1.87E 04	2.58E 04	1.04E 04	2.17E 04
272	43.25	2.10E 04	3.57E 04	1.80E 04	2.47E 04	1.01E 04	2.09E 04
274	44.68	2.02E 04	3.44E 04	1.73E 04	2.36E 04	9.70E 03	2.01E 04
276	46.15	1.94E 04	3.31E 04	1.66E 04	2.26E 04	9.35E 03	1.93E 04
278	47.65	1.87E 04	3.18E 04	1.59E 04	2.16E 04	9.01E 03	1.86E 04
280	49.20	1.80E 04	3.06E 04	1.53E 04	2.07E 04	8.69E 03	1.79E 04
282	50.79	1.73E 04	2.95E 04	1.47E 04	1.98E 04	8.38E 03	1.72E 04
284	52.41	1.67E 04	2.84E 04	1.41E 04	1.89E 04	8.08E 03	1.65E 04
286	54.08	1.61E 04	2.73E 04	1.36E 04	1.81E 04	7.80E 03	1.59E 04
288	55.79	1.55E 04	2.63E 04	1.31E 04	1.74E 04	7.52E 03	1.53E 04
290	57.55	1.49E 04	2.53E 04	1.26E 04	1.66E 04	7.25E 03	1.47E 04
292	59.35	1.43E 04	2.44E 04	1.21E 04	1.59E 04	7.00E 03	1.42E 04
294	61.19	1.38E 04	2.35E 04	1.16E 04	1.53E 04	6.75E 03	1.36E 04
296	63.08	1.33E 04	2.26E 04	1.12E 04	1.46E 04	6.51E 03	1.31E 04
298	65.02	1.28E 04	2.18E 04	1.08E 04	1.40E 04	6.28E 03	1.26E 04

TABLE 2; MASS CONCENTRATION RATIO, MICROGRAM PER GRAM GAS/MICROGRAM PER GRAM LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
300	67.01	1.23E 04	2.10E 04	1.03E 04	1.34E 04	6.06E 03	1.21E 04
302	69.04	1.19E 04	2.02E 04	9.95E 03	1.29E 04	5.85E 03	1.16E 04
304	71.12	1.14E 04	1.95E 04	9.58E 03	1.24E 04	5.64E 03	1.12E 04
306	73.25	1.10E 04	1.88E 04	9.22E 03	1.19E 04	5.45E 03	1.08E 04
308	75.43	1.06E 04	1.81E 04	8.87E 03	1.14E 04	5.26E 03	1.04E 04
310	77.67	1.02E 04	1.74E 04	8.54E 03	1.09E 04	5.07E 03	9.97E 03
312	79.95	9.84E 03	1.68E 04	8.22E 03	1.05E 04	4.90E 03	9.58E 03
314	82.29	9.48E 03	1.62E 04	7.92E 03	1.00E 04	4.73E 03	9.22E 03
316	84.69	9.13E 03	1.56E 04	7.63E 03	9.64E 03	4.56E 03	8.86E 03
318	87.14	8.80E 03	1.50E 04	7.34E 03	9.26E 03	4.41E 03	8.52E 03
320	89.64	8.46E 03	1.45E 04	7.07E 03	8.89E 03	4.26E 03	8.19E 03
322	92.21	8.17E 03	1.40E 04	6.81E 03	8.54E 03	4.11E 03	7.88E 03
324	94.83	7.88E 03	1.35E 04	6.57E 03	8.20E 03	3.97E 03	7.57E 03
326	97.51	7.59E 03	1.30E 04	6.33E 03	7.88E 03	3.83E 03	7.28E 03
328	100.25	7.32E 03	1.25E 04	6.10E 03	7.57E 03	3.70E 03	7.00E 03
330	103.05	7.06E 03	1.21E 04	5.88E 03	7.28E 03	3.57E 03	6.72E 03
332	105.91	6.80E 03	1.17E 04	5.66E 03	6.99E 03	3.45E 03	6.46E 03
334	108.83	6.56E 03	1.13E 04	5.46E 03	6.72E 03	3.33E 03	6.21E 03
336	111.82	6.32E 03	1.09E 04	5.26E 03	6.46E 03	3.22E 03	5.97E 03
338	114.87	6.10E 03	1.05E 04	5.07E 03	6.21E 03	3.11E 03	5.73E 03
340	117.99	5.88E 03	1.01E 04	4.89E 03	5.98E 03	3.01E 03	5.50E 03
342	121.18	5.67E 03	9.75E 03	4.72E 03	5.75E 03	2.90E 03	5.29E 03
344	124.43	5.47E 03	9.41E 03	4.55E 03	5.53E 03	2.81E 03	5.08E 03
346	127.75	5.27E 03	9.08E 03	4.39E 03	5.32E 03	2.71E 03	4.87E 03
348	131.14	5.08E 03	8.76E 03	4.23E 03	5.12E 03	2.62E 03	4.68E 03
350	134.60	4.90E 03	8.46E 03	4.08E 03	4.93E 03	2.53E 03	4.49E 03
352	138.14	4.73E 03	8.16E 03	3.94E 03	4.74E 03	2.45E 03	4.31E 03
354	141.74	4.56E 03	7.88E 03	3.80E 03	4.57E 03	2.37E 03	4.14E 03
356	145.42	4.40E 03	7.60E 03	3.67E 03	4.40E 03	2.29E 03	3.97E 03
358	149.18	4.25E 03	7.34E 03	3.54E 03	4.23E 03	2.21E 03	3.80E 03
360	153.01	4.10E 03	7.09E 03	3.42E 03	4.08E 03	2.14E 03	3.65E 03
362	156.92	3.95E 03	6.84E 03	3.30E 03	3.93E 03	2.07E 03	3.50E 03
364	160.90	3.81E 03	6.61E 03	3.19E 03	3.78E 03	2.00E 03	3.35E 03
366	164.97	3.68E 03	6.38E 03	3.08E 03	3.65E 03	1.93E 03	3.21E 03
368	169.11	3.55E 03	6.16E 03	2.97E 03	3.51E 03	1.87E 03	3.07E 03
370	173.34	3.43E 03	5.95E 03	2.87E 03	3.39E 03	1.81E 03	2.94E 03
372	177.65	3.31E 03	5.74E 03	2.77E 03	3.26E 03	1.75E 03	2.81E 03
374	182.04	3.19E 03	5.55E 03	2.67E 03	3.15E 03	1.69E 03	2.69E 03
376	186.52	3.08E 03	5.36E 03	2.58E 03	3.03E 03	1.63E 03	2.57E 03
378	191.08	2.97E 03	5.18E 03	2.50E 03	2.92E 03	1.58E 03	2.46E 03
380	195.73	2.87E 03	5.00E 03	2.41E 03	2.82E 03	1.53E 03	2.35E 03
382	200.47	2.77E 03	4.83E 03	2.33E 03	2.72E 03	1.48E 03	2.24E 03
384	205.29	2.68E 03	4.66E 03	2.25E 03	2.62E 03	1.43E 03	2.14E 03
386	210.21	2.58E 03	4.51E 03	2.17E 03	2.53E 03	1.38E 03	2.04E 03
388	215.22	2.49E 03	4.35E 03	2.10E 03	2.44E 03	1.34E 03	1.94E 03

TABLE 2; MASS CONCENTRATION RATIO, MICROGRAM PER GRAM GAS/MICROGRAM PER GRAM LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
390	220.32	2.41E 03	4.21E 03	2.03E 03	2.36E 03	1.30E 03	1.84E 03
392	225.52	2.32E 03	4.06E 03	1.96E 03	2.28E 03	1.25E 03	1.75E 03
394	230.81	2.24E 03	3.93E 03	1.90E 03	2.20E 03	1.21E 03	1.66E 03
396	236.18	2.17E 03	3.79E 03	1.83E 03	2.12E 03	1.17E 03	1.58E 03
398	241.68	2.09E 03	3.66E 03	1.77E 03	2.05E 03	1.14E 03	1.49E 03
400	247.28	2.02E 03	3.54E 03	1.71E 03	1.98E 03	1.10E 03	1.41E 03
402	252.94	1.96E 03	3.42E 03	1.66E 03	1.91E 03	1.06E 03	1.33E 03
404	258.73	1.89E 03	3.31E 03	1.60E 03	1.84E 03	1.03E 03	1.25E 03
406	264.61	1.82E 03	3.20E 03	1.55E 03	1.78E 03	9.98E 02	1.17E 03
408	270.60	1.76E 03	3.09E 03	1.50E 03	1.72E 03	9.66E 02	1.09E 03
410	276.69	1.70E 03	2.98E 03	1.45E 03	1.66E 03	9.35E 02	1.01E 03
412	282.88	1.64E 03	2.88E 03	1.40E 03	1.61E 03	9.05E 02	9.30E 02
414	289.20	1.59E 03	2.79E 03	1.35E 03	1.55E 03	8.77E 02	8.40E 02
416	295.62	1.53E 03	2.69E 03	1.31E 03	1.50E 03	8.49E 02	7.24E 02
418	302.14	1.48E 03	2.60E 03	1.27E 03	1.45E 03	8.22E 02	
420	308.78	1.43E 03	2.52E 03	1.23E 03	1.40E 03	7.96E 02	
422	315.53	1.38E 03	2.43E 03	1.19E 03	1.36E 03	7.71E 02	
424	322.39	1.34E 03	2.35E 03	1.15E 03	1.31E 03	7.47E 02	
426	329.37	1.29E 03	2.27E 03	1.11E 03	1.27E 03	7.23E 02	
428	336.46	1.25E 03	2.20E 03	1.07E 03	1.23E 03	7.00E 02	
430	343.67	1.20E 03	2.12E 03	1.04E 03	1.19E 03	6.78E 02	
432	351.00	1.16E 03	2.05E 03	1.01E 03	1.15E 03	6.57E 02	
434	358.46	1.13E 03	1.98E 03	9.73E 02	1.11E 03	6.37E 02	
436	366.03	1.09E 03	1.92E 03	9.41E 02	1.07E 03	6.17E 02	
438	373.72	1.05E 03	1.85E 03	9.11E 02	1.04E 03	5.98E 02	
440	381.54	1.02E 03	1.79E 03	8.82E 02	1.01E 03	5.79E 02	
442	389.49	9.82E 02	1.73E 03	8.54E 02	9.74E 02	5.61E 02	
444	397.56	9.49E 02	1.67E 03	8.26E 02	9.43E 02	5.44E 02	
446	405.76	9.17E 02	1.62E 03	8.00E 02	9.13E 02	5.27E 02	
448	414.09	8.87E 02	1.57E 03	7.74E 02	8.83E 02	5.10E 02	
450	422.56	8.57E 02	1.51E 03	7.50E 02	8.55E 02	4.95E 02	
452	431.14	8.29E 02	1.46E 03	7.26E 02	8.28E 02	4.79E 02	
454	439.87	8.01E 02	1.41E 03	7.03E 02	8.02E 02	4.65E 02	
456	448.73	7.75E 02	1.37E 03	6.80E 02	7.77E 02	4.50E 02	
458	457.73	7.49E 02	1.32E 03	6.59E 02	7.53E 02	4.37E 02	
460	466.87	7.24E 02	1.28E 03	6.38E 02	7.29E 02	4.23E 02	
462	476.14	7.00E 02	1.23E 03	6.17E 02	7.06E 02	4.10E 02	
464	485.56	6.77E 02	1.19E 03	5.98E 02	6.84E 02	3.98E 02	
466	495.12	6.55E 02	1.15E 03	5.79E 02	6.63E 02	3.86E 02	
468	504.83	6.33E 02	1.12E 03	5.61E 02	6.43E 02	3.74E 02	
470	514.68	6.12E 02	1.08E 03	5.43E 02	6.23E 02	3.62E 02	
472	524.67	5.92E 02	1.04E 03	5.26E 02	6.04E 02	3.51E 02	
474	534.81	5.72E 02	1.01E 03	5.09E 02	5.85E 02	3.41E 02	
476	545.11	5.54E 02	9.73E 02	4.93E 02	5.67E 02	3.30E 02	
478	555.55	5.35E 02	9.41E 02	4.78E 02	5.50E 02	3.20E 02	

TABLE 21 MASS CONCENTRATION RATIO, MICROGRAM PER GRAM GAS/MICROGRAM PER GRAM LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
480	566.15	5.18E 02	9.09E 02	4.63E 02	5.33E 02	3.11E 02	
482	576.90	5.01E 02	8.79E 02	4.48E 02	5.17E 02	3.01E 02	
484	587.81	4.84E 02	8.49E 02	4.34E 02	5.01E 02	2.92E 02	
486	598.87	4.68E 02	8.21E 02	4.21E 02	4.86E 02	2.83E 02	
488	610.10	4.53E 02	7.93E 02	4.07E 02	4.71E 02	2.75E 02	
490	621.46	4.38E 02	7.66E 02	3.95E 02	4.57E 02	2.67E 02	
492	633.03	4.24E 02	7.41E 02	3.82E 02	4.44E 02	2.59E 02	
494	644.73	4.10E 02	7.16E 02	3.70E 02	4.30E 02	2.51E 02	
496	656.61	3.97E 02	6.91E 02	3.59E 02	4.17E 02	2.43E 02	
498	668.65	3.84E 02	6.68E 02	3.48E 02	4.05E 02	2.36E 02	
500	680.86	3.71E 02	6.45E 02	3.37E 02	3.93E 02	2.29E 02	
502	693.23	3.59E 02	6.24E 02	3.26E 02	3.81E 02	2.22E 02	
504	705.78	3.47E 02	6.02E 02	3.16E 02	3.70E 02	2.15E 02	
506	718.50	3.36E 02	5.82E 02	3.06E 02	3.59E 02	2.09E 02	
508	731.40	3.25E 02	5.62E 02	2.97E 02	3.49E 02	2.03E 02	
510	744.47	3.14E 02	5.43E 02	2.87E 02	3.38E 02	1.97E 02	
512	757.72	3.04E 02	5.24E 02	2.78E 02	3.28E 02	1.91E 02	
514	771.15	2.94E 02	5.06E 02	2.70E 02	3.19E 02	1.85E 02	
516	784.76	2.85E 02	4.89E 02	2.61E 02	3.10E 02	1.80E 02	
518	798.55	2.76E 02	4.72E 02	2.53E 02	3.00E 02	1.74E 02	
520	812.53	2.67E 02	4.56E 02	2.45E 02	2.92E 02	1.69E 02	
522	826.69	2.58E 02	4.40E 02	2.38E 02	2.83E 02	1.64E 02	
524	841.04	2.49E 02	4.25E 02	2.30E 02	2.75E 02	1.59E 02	
526	855.58	2.41E 02	4.10E 02	2.23E 02	2.67E 02	1.55E 02	
528	870.31	2.34E 02	3.96E 02	2.16E 02	2.59E 02	1.50E 02	
530	885.23	2.26E 02	3.82E 02	2.09E 02	2.52E 02	1.46E 02	
532	900.34	2.19E 02	3.68E 02	2.03E 02	2.45E 02	1.41E 02	
534	915.66	2.12E 02	3.56E 02	1.96E 02	2.38E 02	1.37E 02	
536	931.17	2.05E 02	3.43E 02	1.90E 02	2.31E 02	1.33E 02	
538	946.86	1.98E 02	3.31E 02	1.84E 02	2.24E 02	1.29E 02	
540	962.79	1.92E 02	3.19E 02	1.79E 02	2.18E 02	1.25E 02	
542	978.90	1.85E 02	3.08E 02	1.73E 02	2.12E 02	1.22E 02	
544	995.22	1.79E 02	2.97E 02	1.68E 02	2.06E 02	1.18E 02	
546	1011.75	1.74E 02	2.86E 02	1.62E 02	2.00E 02	1.15E 02	
548	1028.49	1.68E 02	2.76E 02	1.57E 02	1.94E 02	1.11E 02	
550	1045.43	1.62E 02	2.66E 02	1.52E 02	1.89E 02	1.08E 02	
552	1062.59	1.57E 02	2.56E 02	1.48E 02	1.83E 02	1.05E 02	
554	1079.96	1.52E 02	2.47E 02	1.43E 02	1.78E 02	1.02E 02	
556	1097.55	1.47E 02	2.38E 02	1.38E 02	1.73E 02	9.87E 01	
558	1115.36	1.42E 02	2.29E 02	1.34E 02	1.68E 02	9.58E 01	
560	1133.38	1.38E 02	2.21E 02	1.30E 02	1.63E 02	9.30E 01	
562	1151.63	1.33E 02	2.12E 02	1.26E 02	1.59E 02	9.02E 01	
564	1170.10	1.29E 02	2.05E 02	1.22E 02	1.54E 02	8.76E 01	
566	1188.80	1.25E 02	1.97E 02	1.18E 02	1.50E 02	8.50E 01	
568	1207.72	1.21E 02	1.90E 02	1.14E 02	1.46E 02	8.25E 01	

TABLE 2; MASS CONCENTRATION RATIO, MICROGRAM PER GRAM GAS/MICROGRAM PER GRAM LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
570	1226.88	1.17E 02	1 82E 02	1.10E 02	1.42E 02	8.01E 01	
572	1246.26	1.13E 02	1.75E 02	1.07E 02	1.38E 02	7.77E 01	
574	1265.69	1.09E 02	1.69E 02	1.04E 02	1.34E 02	7.54E 01	
576	1285.74	1.06E 02	1.62E 02	1.00E 02	1.30E 02	7.32E 01	
578	1305.84	1.02E 02	1.56E 02	9.70E 01	1.26E 02	7.10E 01	
580	1326.17	9.89E 01	1.50E 02	9.39E 01	1.23E 02	6.89E 01	
582	1346.75	9.56E 01	1.44E 02	9.09E 01	1.19E 02	6.69E 01	
584	1367.57	9.25E 01	1.38E 02	8.80E 01	1.16E 02	6.49E 01	
586	1388.64	8.95E 01	1.33E 02	8.51E 01	1.13E 02	6.30E 01	
588	1409.96	8.65E 01	1.27E 02	8.24E 01	1.10E 02	6.12E 01	
590	1431.52	8.37E 01	1.22E 02	7.97E 01	1.06E 02	5.93E 01	
592	1453.35	8.09E 01	1.17E 02	7.71E 01	1.03E 02	5.76E 01	
594	1475.42	7.83E 01	1.12E 02	7.46E 01	1.01E 02	5.59E 01	
596	1497.76	7.57E 01	1.08E 02	7.22E 01	9.78E 01	5.42E 01	
598	1520.36	7.32E 01	1.03E 02	6.98E 01	9.50E 01	5.26E 01	
600	1543.22	7.08E 01	9.88E 01	6.75E 01	9.23E 01	5.10E 01	

TABLE 31 PARTITION COEFFICIENT, MICROGRAM PER CU.CM. GAS/MICROGRAM PER CU.CM. LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
32	0.09	2.08E 01	4.17E 01	4.55E 01	1.04E 02	4.44E 00	1.76E 01
34	0.10	2.13E 01	4.29E 01	4.60E 01	1.05E 02	4.64E 00	1.83E 01
36	0.10	2.18E 01	4.41E 01	4.65E 01	1.05E 02	4.85E 00	1.90E 01
38	0.11	2.23E 01	4.53E 01	4.70E 01	1.06E 02	5.06E 00	1.96E 01
40	0.12	2.29E 01	4.65E 01	4.75E 01	1.06E 02	5.28E 00	2.03E 01
42	0.13	2.34E 01	4.77E 01	4.79E 01	1.07E 02	5.49E 00	2.09E 01
44	0.14	2.39E 01	4.89E 01	4.83E 01	1.07E 02	5.72E 00	2.15E 01
46	0.15	2.45E 01	5.00E 01	4.88E 01	1.07E 02	5.94E 00	2.22E 01
48	0.17	2.50E 01	5.11E 01	4.91E 01	1.08E 02	6.17E 00	2.28E 01
50	0.18	2.55E 01	5.22E 01	4.95E 01	1.08E 02	6.40E 00	2.34E 01
52	0.19	2.60E 01	5.33E 01	4.98E 01	1.08E 02	6.64E 00	2.40E 01
54	0.21	2.65E 01	5.44E 01	5.02E 01	1.09E 02	6.88E 00	2.47E 01
56	0.22	2.71E 01	5.54E 01	5.05E 01	1.09E 02	7.12E 00	2.53E 01
58	0.24	2.76E 01	5.64E 01	5.08E 01	1.09E 02	7.36E 00	2.59E 01
60	0.26	2.81E 01	5.74E 01	5.10E 01	1.09E 02	7.60E 00	2.64E 01
62	0.27	2.86E 01	5.84E 01	5.13E 01	1.09E 02	7.85E 00	2.70E 01
64	0.29	2.91E 01	5.94E 01	5.15E 01	1.10E 02	8.10E 00	2.76E 01
66	0.32	2.96E 01	6.03E 01	5.17E 01	1.10E 02	8.34E 00	2.82E 01
68	0.34	3.01E 01	6.12E 01	5.19E 01	1.10E 02	8.59E 00	2.87E 01
70	0.36	3.06E 01	6.21E 01	5.21E 01	1.10E 02	8.85E 00	2.93E 01
72	0.39	3.11E 01	6.30E 01	5.23E 01	1.10E 02	9.10E 00	2.98E 01
74	0.42	3.16E 01	6.39E 01	5.24E 01	1.10E 02	9.35E 00	3.03E 01
76	0.44	3.20E 01	6.47E 01	5.25E 01	1.09E 02	9.60E 00	3.09E 01
78	0.47	3.25E 01	6.55E 01	5.26E 01	1.09E 02	9.86E 00	3.14E 01
80	0.51	3.30E 01	6.63E 01	5.27E 01	1.09E 02	1.01E 01	3.19E 01
82	0.54	3.34E 01	6.70E 01	5.28E 01	1.09E 02	1.04E 01	3.24E 01
84	0.58	3.39E 01	6.78E 01	5.29E 01	1.09E 02	1.06E 01	3.29E 01
86	0.62	3.43E 01	6.85E 01	5.30E 01	1.09E 02	1.09E 01	3.33E 01
88	0.66	3.47E 01	6.92E 01	5.30E 01	1.08E 02	1.11E 01	3.38E 01
90	0.70	3.52E 01	6.98E 01	5.30E 01	1.08E 02	1.14E 01	3.43E 01
92	0.74	3.56E 01	7.05E 01	5.31E 01	1.08E 02	1.16E 01	3.47E 01
94	0.79	3.60E 01	7.11E 01	5.31E 01	1.07E 02	1.19E 01	3.52E 01
96	0.84	3.64E 01	7.17E 01	5.31E 01	1.07E 02	1.21E 01	3.56E 01
98	0.89	3.68E 01	7.23E 01	5.30E 01	1.07E 02	1.23E 01	3.60E 01
100	0.95	3.72E 01	7.28E 01	5.30E 01	1.06E 02	1.26E 01	3.64E 01
102	1.01	3.76E 01	7.34E 01	5.30E 01	1.06E 02	1.28E 01	3.68E 01
104	1.07	3.79E 01	7.39E 01	5.29E 01	1.05E 02	1.30E 01	3.72E 01
106	1.13	3.83E 01	7.44E 01	5.28E 01	1.05E 02	1.33E 01	3.75E 01
108	1.20	3.86E 01	7.48E 01	5.28E 01	1.04E 02	1.35E 01	3.79E 01
110	1.27	3.90E 01	7.53E 01	5.27E 01	1.04E 02	1.37E 01	3.83E 01
112	1.35	3.93E 01	7.57E 01	5.26E 01	1.03E 02	1.40E 01	3.86E 01
114	1.43	3.96E 01	7.61E 01	5.25E 01	1.03E 02	1.42E 01	3.89E 01
116	1.51	3.99E 01	7.64E 01	5.24E 01	1.02E 02	1.44E 01	3.93E 01
118	1.60	4.02E 01	7.68E 01	5.22E 01	1.01E 02	1.46E 01	3.96E 01

TABLE 3. PARTITION COEFFICIENT, MICROGRAM PER CU.CM. GAS/MICROGRAM PER CU.CM. LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
120	1.69	4.06E 01	7.71E 01	5.21E 01	1.01E 02	1.48E 01	3.99E 01
122	1.79	4.08E 01	7.74E 01	5.20E 01	1.00E 02	1.50E 01	4.01E 01
124	1.89	4.11E 01	7.77E 01	5.18E 01	9.93E 01	1.52E 01	4.04E 01
126	2.00	4.13E 01	7.80E 01	5.17E 01	9.86E 01	1.54E 01	4.07E 01
128	2.11	4.16E 01	7.83E 01	5.15E 01	9.79E 01	1.56E 01	4.09E 01
130	2.22	4.18E 01	7.85E 01	5.13E 01	9.72E 01	1.58E 01	4.12E 01
132	2.34	4.20E 01	7.87E 01	5.11E 01	9.65E 01	1.60E 01	4.14E 01
134	2.47	4.23E 01	7.89E 01	5.09E 01	9.58E 01	1.62E 01	4.16E 01
136	2.60	4.25E 01	7.91E 01	5.08E 01	9.50E 01	1.63E 01	4.19E 01
138	2.74	4.27E 01	7.92E 01	5.06E 01	9.42E 01	1.65E 01	4.21E 01
140	2.89	4.28E 01	7.94E 01	5.04E 01	9.35E 01	1.67E 01	4.23E 01
142	3.04	4.30E 01	7.95E 01	5.01E 01	9.27E 01	1.68E 01	4.24E 01
144	3.20	4.32E 01	7.96E 01	4.99E 01	9.19E 01	1.70E 01	4.26E 01
146	3.37	4.33E 01	7.97E 01	4.97E 01	9.11E 01	1.71E 01	4.28E 01
148	3.54	4.35E 01	7.97E 01	4.95E 01	9.03E 01	1.73E 01	4.29E 01
150	3.72	4.36E 01	7.98E 01	4.92E 01	8.95E 01	1.74E 01	4.31E 01
152	3.91	4.38E 01	7.98E 01	4.90E 01	8.86E 01	1.75E 01	4.32E 01
154	4.10	4.39E 01	7.99E 01	4.88E 01	8.78E 01	1.77E 01	4.33E 01
156	4.31	4.40E 01	7.99E 01	4.85E 01	8.70E 01	1.78E 01	4.34E 01
158	4.52	4.41E 01	7.98E 01	4.83E 01	8.61E 01	1.79E 01	4.35E 01
160	4.74	4.42E 01	7.98E 01	4.80E 01	8.53E 01	1.80E 01	4.36E 01
162	4.97	4.42E 01	7.98E 01	4.78E 01	8.45E 01	1.81E 01	4.37E 01
164	5.21	4.43E 01	7.97E 01	4.75E 01	8.36E 01	1.82E 01	4.38E 01
166	5.46	4.43E 01	7.96E 01	4.72E 01	8.28E 01	1.83E 01	4.38E 01
168	5.72	4.44E 01	7.96E 01	4.70E 01	8.19E 01	1.84E 01	4.39E 01
170	5.99	4.44E 01	7.95E 01	4.67E 01	8.11E 01	1.85E 01	4.39E 01
172	6.27	4.45E 01	7.94E 01	4.64E 01	8.02E 01	1.86E 01	4.40E 01
174	6.57	4.45E 01	7.92E 01	4.61E 01	7.94E 01	1.87E 01	4.40E 01
176	6.87	4.45E 01	7.91E 01	4.59E 01	7.85E 01	1.88E 01	4.40E 01
178	7.18	4.45E 01	7.89E 01	4.56E 01	7.77E 01	1.88E 01	4.40E 01
180	7.51	4.45E 01	7.88E 01	4.53E 01	7.68E 01	1.89E 01	4.40E 01
182	7.85	4.45E 01	7.86E 01	4.50E 01	7.60E 01	1.90E 01	4.40E 01
184	8.20	4.44E 01	7.84E 01	4.47E 01	7.51E 01	1.90E 01	4.40E 01
186	8.57	4.44E 01	7.82E 01	4.44E 01	7.43E 01	1.91E 01	4.40E 01
188	8.95	4.44E 01	7.80E 01	4.41E 01	7.34E 01	1.91E 01	4.40E 01
190	9.34	4.43E 01	7.78E 01	4.38E 01	7.26E 01	1.92E 01	4.39E 01
192	9.75	4.42E 01	7.76E 01	4.36E 01	7.18E 01	1.92E 01	4.39E 01
194	10.17	4.42E 01	7.73E 01	4.33E 01	7.09E 01	1.92E 01	4.38E 01
196	10.61	4.41E 01	7.71E 01	4.30E 01	7.01E 01	1.93E 01	4.38E 01
198	11.06	4.40E 01	7.68E 01	4.27E 01	6.93E 01	1.93E 01	4.37E 01
200	11.53	4.39E 01	7.66E 01	4.24E 01	6.85E 01	1.93E 01	4.36E 01
202	12.01	4.38E 01	7.63E 01	4.21E 01	6.77E 01	1.93E 01	4.35E 01
204	12.51	4.37E 01	7.60E 01	4.18E 01	6.69E 01	1.93E 01	4.34E 01
206	13.03	4.36E 01	7.57E 01	4.15E 01	6.61E 01	1.93E 01	4.33E 01
208	13.57	4.35E 01	7.54E 01	4.12E 01	6.53E 01	1.93E 01	4.32E 01

TABLE 3;   PARTITION COEFFICIENT, MICROGRAM PER CU.CM. GAS/MICROGRAM PER CU.CM. LIQUID   01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
210	14.12	4.34E 01	7.51E 01	4.09E 01	6.45E 01	1.93E 01	4.31E 01
212	14.70	4.32E 01	7.48E 01	4.06E 01	6.37E 01	1.93E 01	4.30E 01
214	15.29	4.31E 01	7.45E 01	4.03E 01	6.29E 01	1.93E 01	4.29E 01
216	15.90	4.30E 01	7.41E 01	4.00E 01	6.21E 01	1.93E 01	4.27E 01
218	16.53	4.28E 01	7.38E 01	3.96E 01	6.14E 01	1.93E 01	4.26E 01
220	17.19	4.27E 01	7.35E 01	3.93E 01	6.06E 01	1.93E 01	4.24E 01
222	17.86	4.25E 01	7.31E 01	3.90E 01	5.99E 01	1.92E 01	4.23E 01
224	18.56	4.23E 01	7.28E 01	3.87E 01	5.91E 01	1.92E 01	4.21E 01
226	19.27	4.22E 01	7.24E 01	3.84E 01	5.84E 01	1.92E 01	4.20E 01
228	20.01	4.20E 01	7.20E 01	3.81E 01	5.77E 01	1.92E 01	4.18E 01
230	20.78	4.18E 01	7.17E 01	3.78E 01	5.69E 01	1.91E 01	4.16E 01
232	21.57	4.16E 01	7.13E 01	3.75E 01	5.62E 01	1.91E 01	4.14E 01
234	22.38	4.14E 01	7.09E 01	3.72E 01	5.55E 01	1.90E 01	4.13E 01
236	23.22	4.12E 01	7.05E 01	3.69E 01	5.48E 01	1.90E 01	4.11E 01
238	24.08	4.10E 01	7.01E 01	3.66E 01	5.41E 01	1.89E 01	4.09E 01
240	24.97	4.08E 01	6.97E 01	3.63E 01	5.34E 01	1.89E 01	4.07E 01
242	25.88	4.06E 01	6.93E 01	3.60E 01	5.27E 01	1.88E 01	4.05E 01
244	26.83	4.04E 01	6.89E 01	3.57E 01	5.21E 01	1.88E 01	4.02E 01
246	27.80	4.02E 01	6.85E 01	3.54E 01	5.14E 01	1.87E 01	4.00E 01
248	28.80	3.99E 01	6.81E 01	3.52E 01	5.08E 01	1.86E 01	3.98E 01
250	29.82	3.97E 01	6.77E 01	3.49E 01	5.01E 01	1.86E 01	3.96E 01
252	30.88	3.95E 01	6.73E 01	3.46E 01	4.95E 01	1.85E 01	3.94E 01
254	31.97	3.92E 01	6.68E 01	3.43E 01	4.88E 01	1.84E 01	3.91E 01
256	33.09	3.90E 01	6.64E 01	3.40E 01	4.82E 01	1.84E 01	3.89E 01
258	34.24	3.88E 01	6.60E 01	3.37E 01	4.76E 01	1.83E 01	3.86E 01
260	35.43	3.85E 01	6.56E 01	3.34E 01	4.70E 01	1.82E 01	3.84E 01
262	36.64	3.83E 01	6.51E 01	3.31E 01	4.64E 01	1.81E 01	3.81E 01
264	37.89	3.80E 01	6.47E 01	3.28E 01	4.58E 01	1.81E 01	3.79E 01
266	39.18	3.78E 01	6.43E 01	3.25E 01	4.52E 01	1.80E 01	3.76E 01
268	40.50	3.75E 01	6.38E 01	3.23E 01	4.46E 01	1.79E 01	3.74E 01
270	41.86	3.73E 01	6.34E 01	3.20E 01	4.40E 01	1.78E 01	3.71E 01
272	43.25	3.70E 01	6.29E 01	3.17E 01	4.35E 01	1.77E 01	3.68E 01
274	44.68	3.67E 01	6.25E 01	3.14E 01	4.29E 01	1.76E 01	3.65E 01
276	46.15	3.65E 01	6.20E 01	3.11E 01	4.24E 01	1.75E 01	3.63E 01
278	47.65	3.62E 01	6.16E 01	3.09E 01	4.18E 01	1.75E 01	3.60E 01
280	49.20	3.60E 01	6.11E 01	3.06E 01	4.13E 01	1.74E 01	3.57E 01
282	50.79	3.57E 01	6.07E 01	3.03E 01	4.07E 01	1.73E 01	3.54E 01
284	52.41	3.54E 01	6.02E 01	3.00E 01	4.02E 01	1.72E 01	3.51E 01
286	54.08	3.52E 01	5.98E 01	2.98E 01	3.97E 01	1.71E 01	3.48E 01
288	55.79	3.49E 01	5.93E 01	2.95E 01	3.92E 01	1.70E 01	3.45E 01
290	57.55	3.46E 01	5.89E 01	2.92E 01	3.87E 01	1.69E 01	3.42E 01
292	59.35	3.43E 01	5.84E 01	2.90E 01	3.82E 01	1.68E 01	3.39E 01
294	61.19	3.41E 01	5.80E 01	2.87E 01	3.77E 01	1.67E 01	3.36E 01
296	63.08	3.38E 01	5.75E 01	2.84E 01	3.72E 01	1.66E 01	3.33E 01
298	65.02	3.35E 01	5.71E 01	2.82E 01	3.67E 01	1.65E 01	3.30E 01

TABLE 3; PARTITION COEFFICIENT, MICROGRAM PER CU.CM. GAS/MICROGRAM PER CU.CM. LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
300	67.01	3.32E 01	5.66E 01	2.79E 01	3.63E 01	1.64E 01	3.27E 01
302	69.04	3.30E 01	5.62E 01	2.77E 01	3.58E 01	1.63E 01	3.24E 01
304	71.12	3.27E 01	5.57E 01	2.74E 01	3.54E 01	1.62E 01	3.21E 01
306	73.25	3.24E 01	5.53E 01	2.72E 01	3.49E 01	1.60E 01	3.17E 01
308	75.43	3.21E 01	5.48E 01	2.69E 01	3.45E 01	1.59E 01	3.14E 01
310	77.67	3.19E 01	5.44E 01	2.66E 01	3.40E 01	1.58E 01	3.11E 01
312	79.96	3.16E 01	5.39E 01	2.64E 01	3.36E 01	1.57E 01	3.08E 01
314	82.29	3.13E 01	5.35E 01	2.62E 01	3.32E 01	1.56E 01	3.04E 01
316	84.69	3.10E 01	5.30E 01	2.59E 01	3.28E 01	1.55E 01	3.01E 01
318	87.14	3.08E 01	5.26E 01	2.57E 01	3.24E 01	1.54E 01	2.98E 01
320	89.64	3.05E 01	5.21E 01	2.54E 01	3.19E 01	1.53E 01	2.94E 01
322	92.21	3.02E 01	5.17E 01	2.52E 01	3.15E 01	1.52E 01	2.91E 01
324	94.83	2.99E 01	5.12E 01	2.49E 01	3.12E 01	1.51E 01	2.88E 01
326	97.51	2.96E 01	5.08E 01	2.47E 01	3.08E 01	1.50E 01	2.84E 01
328	100.25	2.94E 01	5.03E 01	2.45E 01	3.04E 01	1.48E 01	2.81E 01
330	103.06	2.91E 01	4.99E 01	2.42E 01	3.00E 01	1.47E 01	2.77E 01
332	105.91	2.88E 01	4.94E 01	2.40E 01	2.96E 01	1.46E 01	2.74E 01
334	108.83	2.86E 01	4.90E 01	2.38E 01	2.93E 01	1.45E 01	2.70E 01
336	111.82	2.83E 01	4.86E 01	2.35E 01	2.89E 01	1.44E 01	2.67E 01
338	114.87	2.80E 01	4.81E 01	2.33E 01	2.86E 01	1.43E 01	2.63E 01
340	117.99	2.77E 01	4.77E 01	2.31E 01	2.82E 01	1.42E 01	2.60E 01
342	121.18	2.75E 01	4.72E 01	2.29E 01	2.79E 01	1.41E 01	2.56E 01
344	124.43	2.72E 01	4.68E 01	2.26E 01	2.75E 01	1.40E 01	2.53E 01
346	127.75	2.69E 01	4.64E 01	2.24E 01	2.72E 01	1.39E 01	2.49E 01
348	131.14	2.67E 01	4.60E 01	2.22E 01	2.68E 01	1.37E 01	2.45E 01
350	134.60	2.64E 01	4.55E 01	2.20E 01	2.65E 01	1.36E 01	2.42E 01
352	138.14	2.61E 01	4.51E 01	2.18E 01	2.62E 01	1.35E 01	2.38E 01
354	141.74	2.59E 01	4.47E 01	2.16E 01	2.59E 01	1.34E 01	2.34E 01
356	145.42	2.56E 01	4.42E 01	2.14E 01	2.56E 01	1.33E 01	2.31E 01
358	149.18	2.53E 01	4.38E 01	2.11E 01	2.53E 01	1.32E 01	2.27E 01
360	153.01	2.51E 01	4.34E 01	2.09E 01	2.50E 01	1.31E 01	2.23E 01
362	156.92	2.48E 01	4.30E 01	2.07E 01	2.47E 01	1.30E 01	2.20E 01
364	160.90	2.46E 01	4.26E 01	2.05E 01	2.44E 01	1.29E 01	2.16E 01
366	164.97	2.43E 01	4.22E 01	2.03E 01	2.41E 01	1.28E 01	2.12E 01
368	169.11	2.41E 01	4.17E 01	2.01E 01	2.38E 01	1.27E 01	2.08E 01
370	173.34	2.38E 01	4.13E 01	1.99E 01	2.35E 01	1.25E 01	2.04E 01
372	177.65	2.36E 01	4.09E 01	1.97E 01	2.32E 01	1.24E 01	2.00E 01
374	182.04	2.33E 01	4.05E 01	1.95E 01	2.30E 01	1.23E 01	1.96E 01
376	186.52	2.31E 01	4.01E 01	1.93E 01	2.27E 01	1.22E 01	1.93E 01
378	191.08	2.28E 01	3.97E 01	1.91E 01	2.24E 01	1.21E 01	1.89E 01
380	195.73	2.26E 01	3.93E 01	1.90E 01	2.22E 01	1.20E 01	1.85E 01
382	200.47	2.23E 01	3.89E 01	1.88E 01	2.19E 01	1.19E 01	1.80E 01
384	205.29	2.21E 01	3.85E 01	1.86E 01	2.17E 01	1.18E 01	1.76E 01
386	210.21	2.19E 01	3.81E 01	1.84E 01	2.14E 01	1.17E 01	1.72E 01
388	215.22	2.16E 01	3.77E 01	1.82E 01	2.12E 01	1.16E 01	1.68E 01

TABLE 6; PARTITION COEFFICIENT, MICROGRAM PER CU.CM. GAS/MICROGRAM PER CU.CM. LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
390	220.32	2.14E 01	3.73E 01	1.80E 01	2.09E 01	1.15E 01	1.64E 01
392	225.52	2.11E 01	3.70E 01	1.78E 01	2.07E 01	1.14E 01	1.59E 01
394	230.81	2.09E 01	3.66E 01	1.77E 01	2.05E 01	1.13E 01	1.55E 01
396	236.19	2.07E 01	3.62E 01	1.75E 01	2.02E 01	1.12E 01	1.50E 01
398	241.68	2.05F 01	3.58E 01	1.73E 01	2.00E 01	1.11E 01	1.46E 01
400	247.26	2.02E 01	3.54E 01	1.71E 01	1.98E 01	1.10E 01	1.41E 01
402	252.94	2.00E 01	3.51E 01	1.70E 01	1.96E 01	1.09E 01	1.36E 01
404	258.73	1.98E 01	3.47E 01	1.68E 01	1.93E 01	1.08E 01	1.31E 01
406	264.61	1.96E 01	3.43E 01	1.66E 01	1.91E 01	1.07E 01	1.26E 01
408	270.60	1.93E 01	3.39E 01	1.65E 01	1.89E 01	1.06E 01	1.20E 01
410	276.69	1.91E 01	3.36E 01	1.63E 01	1.87E 01	1.05E 01	1.14E 01
412	282.89	1.89E 01	3.32E 01	1.61E 01	1.85E 01	1.04E 01	1.07E 01
414	289.20	1.87E 01	3.28E 01	1.60E 01	1.83E 01	1.03E 01	9.90E 00
416	295.62	1.85E 01	3.25E 01	1.58E 01	1.81E 01	1.02E 01	8.73E 00
418	302.14	1.83E 01	3.21E 01	1.56E 01	1.79E 01	1.01E 01	
420	308.78	1.81E 01	3.18E 01	1.55E 01	1.77E 01	1.00E 01	
422	315.53	1.79E 01	3.14E 01	1.53E 01	1.75E 01	9.96E 00	
424	322.39	1.76E 01	3.11E 01	1.52E 01	1.73E 01	9.87E 00	
426	329.37	1.74E 01	3.07E 01	1.50E 01	1.71E 01	9.78E 00	
428	336.46	1.72E 01	3.04E 01	1.48E 01	1.70E 01	9.69E 00	
430	343.67	1.70E 01	3.00E 01	1.47E 01	1.68E 01	9.60E 00	
432	351.00	1.68E 01	2.97E 01	1.45E 01	1.66E 01	9.51E 00	
434	358.46	1.67E 01	2.94E 01	1.44E 01	1.64E 01	9.42E 00	
436	366.03	1.65E 01	2.90E 01	1.42E 01	1.63E 01	9.33E 00	
438	373.72	1.63E 01	2.87E 01	1.41E 01	1.61E 01	9.25E 00	
440	381.54	1.61E 01	2.84E 01	1.40E 01	1.59E 01	9.16E 00	
442	389.49	1.59E 01	2.80E 01	1.38E 01	1.58E 01	9.08E 00	
444	397.56	1.57E 01	2.77E 01	1.37E 01	1.56E 01	8.99E 00	
446	405.76	1.55E 01	2.74E 01	1.35E 01	1.54E 01	8.91E 00	
448	414.09	1.53E 01	2.71E 01	1.34E 01	1.53E 01	8.83E 00	
450	422.55	1.52E 01	2.68E 01	1.33E 01	1.51E 01	8.75E 00	
452	431.14	1.50E 01	2.64E 01	1.31E 01	1.50E 01	8.67E 00	
454	439.87	1.48E 01	2.61E 01	1.30E 01	1.48E 01	8.58E 00	
456	448.73	1.46E 01	2.58E 01	1.28E 01	1.47E 01	8.50E 00	
458	457.73	1.45E 01	2.55E 01	1.27E 01	1.46E 01	8.43E 00	
460	466.87	1.43E 01	2.52E 01	1.26E 01	1.44E 01	8.35E 00	
462	476.14	1.41E 01	2.49E 01	1.24E 01	1.42E 01	8.27E 00	
464	485.56	1.39E 01	2.46E 01	1.23E 01	1.41E 01	8.19E 00	
466	495.12	1.38E 01	2.43E 01	1.22E 01	1.40E 01	8.12E 00	
468	504.83	1.36E 01	2.40E 01	1.21E 01	1.38E 01	8.04E 00	
470	514.67	1.35E 01	2.37E 01	1.19E 01	1.37E 01	7.97E 00	
472	524.67	1.33E 01	2.34E 01	1.18E 01	1.36E 01	7.89E 00	
474	534.81	1.31E 01	2.31E 01	1.17E 01	1.34E 01	7.82E 00	
476	545.11	1.30E 01	2.28E 01	1.16E 01	1.33E 01	7.75E 00	
478	555.55	1.28E 01	2.25E 01	1.14E 01	1.32E 01	7.67E 00	

TABLE 01 PARTITION COEFFICIENT, MICROGRAM PER CU.CM. GAS/MICROGRAM PER CU.CM. LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
480	566.15	1.27E 01	2.23E 01	1.13E 01	1.30E 01	7.60E 00	
482	576.90	1.25E 01	2.20E 01	1.12E 01	1.29E 01	7.53E 00	
484	587.81	1.24E 01	2.17E 01	1.11E 01	1.28E 01	7.46E 00	
486	598.87	1.22E 01	2.14E 01	1.10E 01	1.27E 01	7.39E 00	
488	610.10	1.21E 01	2.11E 01	1.09E 01	1.26E 01	7.33E 00	
490	621.46	1.19E 01	2.09E 01	1.07E 01	1.25E 01	7.26E 00	
492	633.03	1.18E 01	2.06E 01	1.06E 01	1.23E 01	7.19E 00	
494	644.73	1.16E 01	2.03E 01	1.05E 01	1.22E 01	7.12E 00	
496	656.61	1.15E 01	2.01E 01	1.04E 01	1.21E 01	7.06E 00	
498	668.65	1.14E 01	1.98E 01	1.03E 01	1.20E 01	6.99E 00	
500	680.86	1.12E 01	1.95E 01	1.02E 01	1.19E 01	6.93E 00	
502	693.23	1.11E 01	1.93E 01	1.01E 01	1.18E 01	6.87E 00	
504	705.76	1.10E 01	1.90E 01	9.98E 00	1.17E 01	6.80E 00	
506	718.50	1.08E 01	1.88E 01	9.87E 00	1.16E 01	6.74E 00	
508	731.40	1.07E 01	1.85E 01	9.77E 00	1.15E 01	6.68E 00	
510	744.47	1.06E 01	1.83E 01	9.67E 00	1.14E 01	6.62E 00	
512	757.72	1.05E 01	1.80E 01	9.57E 00	1.13E 01	6.56E 00	
514	771.15	1.03E 01	1.78E 01	9.46E 00	1.12E 01	6.50E 00	
516	784.76	1.02E 01	1.75E 01	9.36E 00	1.11E 01	6.44E 00	
518	798.55	1.01E 01	1.73E 01	9.26E 00	1.10E 01	6.38E 00	
520	812.53	9.96E 00	1.70E 01	9.17E 00	1.09E 01	6.32E 00	
522	826.69	9.84E 00	1.68E 01	9.07E 00	1.08E 01	6.27E 00	
524	841.04	9.73E 00	1.66E 01	8.97E 00	1.07E 01	6.21E 00	
526	855.58	9.61E 00	1.63E 01	8.88E 00	1.06E 01	6.15E 00	
528	870.31	9.49E 00	1.61E 01	8.78E 00	1.05E 01	6.10E 00	
530	885.23	9.38E 00	1.59E 01	8.69E 00	1.05E 01	6.04E 00	
532	900.34	9.27E 00	1.56E 01	8.60E 00	1.04E 01	5.99E 00	
534	915.66	9.16E 00	1.54E 01	8.51E 00	1.03E 01	5.94E 00	
536	931.17	9.05E 00	1.52E 01	8.42E 00	1.02E 01	5.89E 00	
538	946.88	8.94E 00	1.49E 01	8.33E 00	1.01E 01	5.83E 00	
540	962.79	8.84E 00	1.47E 01	8.24E 00	1.00E 01	5.78E 00	
542	978.90	8.73E 00	1.45E 01	8.15E 00	9.97E 00	5.73E 00	
544	995.22	8.63E 00	1.43E 01	8.06E 00	9.89E 00	5.68E 00	
546	1011.75	8.53E 00	1.41E 01	7.98E 00	9.81E 00	5.63E 00	
548	1028.49	8.43E 00	1.38E 01	7.89E 00	9.74E 00	5.58E 00	
550	1045.43	8.33E 00	1.36E 01	7.81E 00	9.66E 00	5.53E 00	
552	1062.59	8.23E 00	1.34E 01	7.72E 00	9.59E 00	5.49E 00	
554	1079.96	8.13E 00	1.32E 01	7.64E 00	9.52E 00	5.44E 00	
556	1097.55	8.04E 00	1.30E 01	7.56E 00	9.45E 00	5.39E 00	
558	1115.38	7.94E 00	1.28E 01	7.48E 00	9.38E 00	5.35E 00	
560	1133.[illegible]3	7.85E 00	1.26E 01	7.40E 00	9.31E 00	5.30E 00	
562	1151.63	7.76E 00	1.24E 01	7.32E 00	9.24E 00	5.26E 00	
564	1170.10	7.67E 00	1.22E 01	7.24E 00	9.18E 00	5.21E 00	
566	1188.80	7.58E 00	1.20E 01	7.16E 00	9.11E 00	5.17E 00	
568	1207.72	7.49E 00	1.18E 01	7.09E 00	9.05E 00	5.12E 00	

TABLE 3; PARTITION COEFFICIENT, MICROGRAM PER CU.CM. GAS/MICROGRAM PER CU.CM. LIQUID 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
570	1226.88	7.41E 00	1.16E 01	7.01E 00	8.99E 00	5.08E 00	
572	1246.26	7.32E 00	1.14E 01	6.94E 00	8.92E 00	5.04E 00	
574	1265.89	7.24E 00	1.12E 01	6.86E 00	8.86E 00	5.00E 00	
576	1285.74	7.16E 00	1.10E 01	6.79E 00	8.80E 00	4.96E 00	
578	1305.84	7.07E 00	1.08E 01	6.72E 00	8.74E 00	4.92E 00	
580	1326.17	6.99E 00	1.06E 01	6.64E 00	8.68E 00	4.88E 00	
582	1346.75	6.91E 00	1.04E 01	6.57E 00	8.63E 00	4.84E 00	
584	1367.57	6.84E 00	1.02E 01	6.50E 00	8.57E 00	4.80E 00	
586	1388.64	6.76E 00	1.00E 01	6.43E 00	8.52E 00	4.76E 00	
588	1409.96	6.68E 00	9.84E 00	6.36E 00	8.46E 00	4.72E 00	
590	1431.52	6.61E 00	9.65E 00	6.30E 00	8.41E 00	4.69E 00	
592	1453.35	6.54E 00	9.46E 00	6.23E 00	8.36E 00	4.65E 00	
594	1475.42	6.46E 00	9.28E 00	6.16E 00	8.31E 00	4.61E 00	
596	1497.76	6.39E 00	9.09E 00	6.10E 00	8.26E 00	4.58E 00	
598	1520.36	6.32E 00	8.91E 00	6.03E 00	8.21E 00	4.54E 00	
600	1543.22	6.25E 00	8.73E 00	5.97E 00	8.16E 00	4.51E 00	

TABLE 4;

HENRYS LAW CONSTANT, ATM/MOLE FRACTION

01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
32	0.09	2.58E 04	5.19E 04	5.66E 04	1.29E 05	5.53E 03	2.20E 04
34	0.10	2.66E 04	5.36E 04	5.75E 04	1.31E 05	5.80E 03	2.29E 04
36	0.10	2.74E 04	5.54E 04	5.84E 04	1.32E 05	6.08E 03	2.38E 04
38	0.11	2.81E 04	5.71E 04	5.92E 04	1.33E 05	6.38E 03	2.47E 04
40	0.12	2.89E 04	5.88E 04	6.01E 04	1.34E 05	6.67E 03	2.56E 04
42	0.13	2.97E 04	6.06E 04	6.09E 04	1.35E 05	6.98E 03	2.65E 04
44	0.14	3.05E 04	6.23E 04	6.16E 04	1.36E 05	7.29E 03	2.75E 04
46	0.15	3.13E 04	6.40E 04	6.24E 04	1.37E 05	7.60E 03	2.84E 04
48	0.17	3.21E 04	6.57E 04	6.31E 04	1.38E 05	7.93E 03	2.93E 04
50	0.18	3.29E 04	6.73E 04	6.38E 04	1.39E 05	8.26E 03	3.02E 04
52	0.19	3.37E 04	6.90E 04	6.45E 04	1.40E 05	8.59E 03	3.11E 04
54	0.21	3.45E 04	7.06E 04	6.52E 04	1.41E 05	8.93E 03	3.20E 04
56	0.22	3.53E 04	7.23E 04	6.58E 04	1.42E 05	9.28E 03	3.29E 04
58	0.24	3.61E 04	7.39E 04	6.64E 04	1.43E 05	9.63E 03	3.38E 04
60	0.26	3.69E 04	7.55E 04	6.70E 04	1.44E 05	9.99E 03	3.47E 04
62	0.27	3.77E 04	7.70E 04	6.76E 04	1.44E 05	1.04E 04	3.56E 04
64	0.29	3.85E 04	7.86E 04	6.82E 04	1.45E 05	1.07E 04	3.65E 04
66	0.32	3.93E 04	8.01E 04	6.87E 04	1.46E 05	1.11E 04	3.74E 04
68	0.34	4.01E 04	8.16E 04	6.92E 04	1.46E 05	1.15E 04	3.83E 04
70	0.36	4.09E 04	8.31E 04	6.97E 04	1.47E 05	1.18E 04	3.92E 04
72	0.39	4.17E 04	8.46E 04	7.02E 04	1.47E 05	1.22E 04	4.00E 04
74	0.42	4.25E 04	8.60E 04	7.06E 04	1.48E 05	1.26E 04	4.09E 04
76	0.44	4.33E 04	8.75E 04	7.10E 04	1.48E 05	1.30E 04	4.17E 04
78	0.47	4.41E 04	8.89E 04	7.14E 04	1.48E 05	1.34E 04	4.26E 04
80	0.51	4.49E 04	9.02E 04	7.18E 04	1.49E 05	1.38E 04	4.34E 04
82	0.54	4.57E 04	9.16E 04	7.22E 04	1.49E 05	1.42E 04	4.42E 04
84	0.58	4.64E 04	9.29E 04	7.25E 04	1.49E 05	1.45E 04	4.51E 04
86	0.62	4.72E 04	9.42E 04	7.28E 04	1.49E 05	1.49E 04	4.59E 04
88	0.66	4.79E 04	9.54E 04	7.31E 04	1.49E 05	1.53E 04	4.67E 04
90	0.70	4.87E 04	9.67E 04	7.34E 04	1.50E 05	1.57E 04	4.74E 04
92	0.74	4.94E 04	9.79E 04	7.37E 04	1.50E 05	1.61E 04	4.82E 04
94	0.79	5.02E 04	9.91E 04	7.39E 04	1.50E 05	1.65E 04	4.90E 04
96	0.84	5.09E 04	1.00E 05	7.42E 04	1.50E 05	1.69E 04	4.97E 04
98	0.89	5.16E 04	1.01E 05	7.44E 04	1.49E 05	1.73E 04	5.05E 04
100	0.95	5.23E 04	1.02E 05	7.46E 04	1.49E 05	1.77E 04	5.12E 04
102	1.01	5.30E 04	1.04E 05	7.47E 04	1.49E 05	1.81E 04	5.19E 04
104	1.07	5.37E 04	1.05E 05	7.49E 04	1.49E 05	1.85E 04	5.26E 04
106	1.13	5.44E 04	1.06E 05	7.50E 04	1.49E 05	1.89E 04	5.33E 04
108	1.20	5.50E 04	1.07E 05	7.52E 04	1.48E 03	1.92E 04	5.40E 04
110	1.27	5.57E 04	1.08E 05	7.53E 04	1.48E 05	1.96E 04	5.47E 04
112	1.35	5.63E 04	1.08E 05	7.54E 04	1.48E 05	2.00E 04	5.53E 04
114	1.43	5.70E 04	1.09E 05	7.54E 04	1.47E 05	2.04E 04	5.60E 04
116	1.51	5.76E 04	1.10E 05	7.55E 04	1.47E 05	2.08E 04	5.66E 04
118	1.60	5.82E 04	1.11E 05	7.55E 04	1.46E 05	2.11E 04	5.72E 04

TABLE 4; HENRYS LAW CONSTANT, ATM/MOLE FRACTION 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
120	1.69	5.88E 04	1.12E 05	7.56E 04	1.46E 05	2.15E 04	5.78E 04
122	1.79	5.93E 04	1.13E 05	7.56E 04	1.45E 05	2.18E 04	5.84E 04
124	1.89	5.99E 04	1.13E 05	7.56E 04	1.45E 05	2.22E 04	5.90E 04
126	2.00	6.05E 04	1.14E 05	7.56E 04	1.44E 05	2.26E 04	5.95E 04
128	2.11	6.10E 04	1.15E 05	7.56E 04	1.44E 05	2.29E 04	6.01E 04
130	2.22	6.15E 04	1.16E 05	7.55E 04	1.43E 05	2.32E 04	6.06E 04
132	2.34	6.20E 04	1.16E 05	7.55E 04	1.42E 05	2.36E 04	6.11E 04
134	2.47	6.25E 04	1.17E 05	7.54E 04	1.42E 05	2.39E 04	6.16E 04
136	2.60	6.30E 04	1.17E 05	7.53E 04	1.41E 05	2.42E 04	6.21E 04
138	2.74	6.35E 04	1.18E 05	7.52E 04	1.40E 05	2.45E 04	6.26E 04
140	2.89	6.39E 04	1.18E 05	7.51E 04	1.39E 05	2.49E 04	6.31E 04
142	3.04	6.44E 04	1.19E 05	7.50E 04	1.39E 05	2.52E 04	6.35E 04
144	3.20	6.48E 04	1.19E 05	7.49E 04	1.38E 05	2.55E 04	6.39E 04
146	3.37	6.52E 04	1.20E 05	7.48E 04	1.37E 05	2.58E 04	6.44E 04
148	3.54	6.56E 04	1.20E 05	7.46E 04	1.36E 05	2.61E 04	6.48E 04
150	3.72	6.60E 04	1.21E 05	7.45E 04	1.35E 05	2.63E 04	6.51E 04
152	3.91	6.64E 04	1.21E 05	7.43E 04	1.34E 05	2.66E 04	6.55E 04
154	4.10	6.67E 04	1.21E 05	7.41E 04	1.34E 05	2.69E 04	6.59E 04
156	4.31	6.70E 04	1.22E 05	7.40E 04	1.33E 05	2.71E 04	6.62E 04
158	4.52	6.74E 04	1.22E 05	7.38E 04	1.32E 05	2.74E 04	6.65E 04
160	4.74	6.77E 04	1.22E 05	7.36E 04	1.31E 05	2.76E 04	6.69E 04
162	4.97	6.80E 04	1.23E 05	7.34E 04	1.30E 05	2.79E 04	6.71E 04
164	5.21	6.82E 04	1.23E 05	7.32E 04	1.29E 05	2.81E 04	6.74E 04
166	5.46	6.85E 04	1.23E 05	7.29E 04	1.28E 05	2.83E 04	6.77E 04
168	5.72	6.87E 04	1.23E 05	7.27E 04	1.27E 05	2.86E 04	6.80E 04
170	5.99	6.90E 04	1.23E 05	7.25E 04	1.26E 05	2.88E 04	6.82E 04
172	6.27	6.92E 04	1.23E 05	7.22E 04	1.25E 05	2.90E 04	6.84E 04
174	6.57	6.94E 04	1.24E 05	7.20E 04	1.24E 05	2.92E 04	6.86E 04
176	6.87	6.96E 04	1.24E 05	7.17E 04	1.23E 05	2.94E 04	6.88E 04
178	7.18	6.97E 04	1.24E 05	7.14E 04	1.22E 05	2.95E 04	6.90E 04
180	7.51	6.99E 04	1.24E 05	7.12E 04	1.21E 05	2.97E 04	6.92E 04
182	7.85	7.00E 04	1.24E 05	7.09E 04	1.20E 05	2.99E 04	6.93E 04
184	8.20	7.01E 04	1.24E 05	7.06E 04	1.19E 05	3.00E 04	6.95E 04
186	8.57	7.03E 04	1.24E 05	7.03E 04	1.18E 05	3.02E 04	6.96E 04
188	8.95	7.03E 04	1.24E 05	7.00E 04	1.16E 05	3.03E 04	6.97E 04
190	9.34	7.04E 04	1.24E 05	6.97E 04	1.15E 05	3.05E 04	6.98E 04
192	9.75	7.05E 04	1.24E 05	6.94E 04	1.14E 05	3.06E 04	6.99E 04
194	10.17	7.06E 04	1.24E 05	6.91E 04	1.13E 05	3.07E 04	7.00E 04
196	10.61	7.06E 04	1.23E 05	6.88E 04	1.12E 05	3.08E 04	7.00E 04
198	11.06	7.06E 04	1.23E 05	6.84E 04	1.11E 05	3.09E 04	7.01E 04
200	11.53	7.06E 04	1.23E 05	6.81E 04	1.10E 05	3.10E 04	7.01E 04
202	12.01	7.06E 04	1.23E 05	6.78E 04	1.09E 05	3.11E 04	7.01E 04
204	12.51	7.06E 04	1.23E 05	6.74E 04	1.08E 05	3.12E 04	7.01E 04
206	13.03	7.06E 04	1.23E 05	6.71E 04	1.07E 05	3.13E 04	7.01E 04
208	13.57	7.06E 04	1.22E 05	6.68E 04	1.06E 05	3.14E 04	7.01E 04

TABLE 4; HENRYS LAW CONSTANT, ATM/MOLE FRACTION 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
210	14.12	7.06E 04	1.22E 05	6.64E 04	1.05E 05	3.14E 04	7.01E 04
212	14.70	7.04E 04	1.22E 05	6.61E 04	1.04E 05	3.15E 04	7.00E 04
214	15.29	7.04E 04	1.22E 05	6.57E 04	1.03E 05	3.15E 04	7.00E 04
216	15.90	7.03E 04	1.21E 05	6.54E 04	1.02E 05	3.16E 04	6.99E 04
218	16.53	7.02E 04	1.21E 05	6.50E 04	1.01E 05	3.16E 04	6.98E 04
220	17.19	7.01E 04	1.21E 05	6.46E 04	9.96E 04	3.17E 04	6.97E 04
222	17.86	7.00E 04	1.20E 05	6.43E 04	9.86E 04	3.17E 04	6.96E 04
224	18.56	6.98E 04	1.20E 05	6.39E 04	9.75E 04	3.17E 04	6.95E 04
226	19.27	6.97E 04	1.20E 05	6.35E 04	9.65E 04	3.17E 04	6.94E 04
228	20.01	6.95E 04	1.19E 05	6.32E 04	9.55E 04	3.17E 04	6.92E 04
230	20.78	6.94E 04	1.19E 05	6.28E 04	9.45E 04	3.17E 04	6.91E 04
232	21.57	6.92E 04	1.19E 05	6.24E 04	9.35E 04	3.17E 04	6.89E 04
234	22.38	6.90E 04	1.18E 05	6.20E 04	9.25E 04	3.17E 04	6.88E 04
236	23.22	6.88E 04	1.18E 05	6.17E 04	9.15E 04	3.17E 04	6.86E 04
238	24.08	6.86E 04	1.17E 05	6.13E 04	9.05E 04	3.17E 04	6.84E 04
240	24.97	6.84E 04	1.17E 05	6.09E 04	8.95E 04	3.17E 04	6.82E 04
242	25.88	6.82E 04	1.16E 05	6.05E 04	8.86E 04	3.16E 04	6.79E 04
244	26.83	6.79E 04	1.16E 05	6.01E 04	8.76E 04	3.16E 04	6.77E 04
246	27.80	6.77E 04	1.15E 05	5.98E 04	8.67E 04	3.15E 04	6.75E 04
248	28.80	6.74E 04	1.15E 05	5.94E 04	8.57E 04	3.15E 04	6.72E 04
250	29.82	6.72E 04	1.15E 05	5.90E 04	8.48E 04	3.14E 04	6.70E 04
252	30.88	6.69E 04	1.14E 05	5.86E 04	8.39E 04	3.14E 04	6.67E 04
254	31.97	6.66E 04	1.14E 05	5.82E 04	8.29E 04	3.13E 04	6.64E 04
256	33.09	6.64E 04	1.13E 05	5.78E 04	8.20E 04	3.13E 04	6.62E 04
258	34.24	6.61E 04	1.12E 05	5.74E 04	8.11E 04	3.12E 04	6.59E 04
260	35.43	6.58E 04	1.12E 05	5.70E 04	8.02E 04	3.11E 04	6.56E 04
262	36.64	6.55E 04	1.11E 05	5.67E 04	7.93E 04	3.10E 04	6.52E 04
264	37.89	6.52E 04	1.11E 05	5.63E 04	7.84E 04	3.10E 04	6.49E 04
266	39.18	6.49E 04	1.10E 05	5.59E 04	7.76E 04	3.09E 04	6.46E 04
268	40.50	6.45E 04	1.10E 05	5.55E 04	7.67E 04	3.08E 04	6.42E 04
270	41.86	6.42E 04	1.09E 05	5.51E 04	7.58E 04	3.07E 04	6.39E 04
272	43.25	6.39E 04	1.09E 05	5.47E 04	7.50E 04	3.06E 04	6.35E 04
274	44.68	6.35E 04	1.08E 05	5.43E 04	7.42E 04	3.05E 04	6.32E 04
276	46.15	6.32E 04	1.07E 05	5.39E 04	7.33E 04	3.04E 04	6.28E 04
278	47.65	6.28E 04	1.07E 05	5.35E 04	7.25E 04	3.03E 04	6.24E 04
280	49.20	6.25E 04	1.06E 05	5.31E 04	7.17E 04	3.02E 04	6.20E 04
282	50.79	6.21E 04	1.06E 05	5.27E 04	7.09E 04	3.00E 04	6.16E 04
284	52.41	6.17E 04	1.05E 05	5.24E 04	7.01E 04	2.99E 04	6.12E 04
286	54.08	6.14E 04	1.04E 05	5.20E 04	6.93E 04	2.98E 04	6.08E 04
288	55.79	6.10E 04	1.04E 05	5.16E 04	6.85E 04	2.97E 04	6.04E 04
290	57.55	6.06E 04	1.03E 05	5.12E 04	6.78E 04	2.96E 04	6.00E 04
292	59.35	6.02E 04	1.03E 05	5.08E 04	6.70E 04	2.94E 04	5.95E 04
294	61.19	5.99E 04	1.02E 05	5.04E 04	6.62E 04	2.93E 04	5.91E 04
296	63,08	5.95E 04	1.01E 05	5.00E 04	6.55E 04	2.92E 04	5.86E 04
298	65,02	5.91E 04	1.01E 05	4.97E 04	6.48E 04	2.90E 04	5.82E 04

TABLE 4; HENRYS LAW CONSTANT, ATM/MOLE FRACTION 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
300	67.01	5.87E 04	1.00E 05	4.93E 04	6.40E 04	2.89E 04	5.77E 04
302	69.04	5.83E 04	9.93E 04	4.89E 04	6.33E 04	2.87E 04	5.72E 04
304	71.12	5.79E 04	9.86E 04	4.85E 04	6.26E 04	2.86E 04	5.68E 04
306	73.25	5.75E 04	9.80E 04	4.81E 04	6.19E 04	2.84E 04	5.63E 04
308	75.43	5.71E 04	9.73E 04	4.78E 04	6.12E 04	2.83E 04	5.58E 04
310	77.67	5.67E 04	9.67E 04	4.74E 04	6.05E 04	2.82E 04	5.53E 04
312	79.95	5.62E 04	9.60E 04	4.70E 04	5.98E 04	2.80E 04	5.48E 04
314	82.29	5.58E 04	9.53E 04	4.66E 04	5.92E 04	2.78E 04	5.43E 04
316	84.69	5.54E 04	9.47E 04	4.63E 04	5.85E 04	2.77E 04	5.38E 04
318	87.14	5.50E 04	9.40E 04	4.59E 04	5.79E 04	2.75E 04	5.32E 04
320	89.64	5.46E 04	9.33E 04	4.55E 04	5.72E 04	2.74E 04	5.27E 04
322	92.21	5.42E 04	9.26E 04	4.51E 04	5.66E 04	2.72E 04	5.22E 04
324	94.83	5.37E 04	9.20E 04	4.48E 04	5.59E 04	2.71E 04	5.16E 04
326	97.51	5.33E 04	9.13E 04	4.44E 04	5.53E 04	2.69E 04	5.11E 04
328	100.25	5.29E 04	9.06E 04	4.40E 04	5.47E 04	2.67E 04	5.05E 04
330	103.06	5.25E 04	8.99E 04	4.37E 04	5.41E 04	2.66E 04	5.00E 04
332	105.91	5.20E 04	8.92E 04	4.33E 04	5.35E 04	2.64E 04	4.94E 04
334	108.83	5.16E 04	8.86E 04	4.30E 04	5.29E 04	2.62E 04	4.89E 04
336	111.82	5.12E 04	8.79E 04	4.26E 04	5.23E 04	2.61E 04	4.83E 04
338	114.87	5.07E 04	8.72E 04	4.22E 04	5.17E 04	2.59E 04	4.77E 04
340	117.99	5.03E 04	8.65E 04	4.19E 04	5.12E 04	2.57E 04	4.71E 04
342	121.18	4.99E 04	8.58E 04	4.15E 04	5.06E 04	2.56E 04	4.65E 04
344	124.43	4.95E 04	8.51E 04	4.12E 04	5.00E 04	2.54E 04	4.59E 04
346	127.75	4.90E 04	8.45E 04	4.08E 04	4.95E 04	2.52E 04	4.53E 04
348	131.14	4.86E 04	8.38E 04	4.05E 04	4.89E 04	2.51E 04	4.47E 04
350	134.60	4.82E 04	8.31E 04	4.01E 04	4.84E 04	2.49E 04	4.41E 04
352	138.14	4.77E 04	8.24E 04	3.98E 04	4.79E 04	2.47E 04	4.35E 04
354	141.74	4.73E 04	8.17E 04	3.94E 04	4.74E 04	2.45E 04	4.29E 04
356	145.42	4.69E 04	8.10E 04	3.91E 04	4.68E 04	2.44E 04	4.23E 04
358	149.18	4.65E 04	8.03E 04	3.88E 04	4.63E 04	2.42E 04	4.16E 04
360	153.01	4.60E 04	7.97E 04	3.84E 04	4.58E 04	2.40E 04	4.10E 04
362	156.92	4.56E 04	7.90E 04	3.81E 04	4.53E 04	2.38E 04	4.03E 04
364	160.90	4.52E 04	7.83E 04	3.78E 04	4.48E 04	2.37E 04	3.97E 04
366	164.97	4.48E 04	7.76E 04	3.74E 04	4.44E 04	2.35E 04	3.90E 04
368	169.11	4.44E 04	7.69E 04	3.71E 04	4.39E 04	2.33E 04	3.84E 04
370	173.34	4.39E 04	7.63E 04	3.68E 04	4.34E 04	2.32E 04	3.77E 04
372	177.65	4.35E 04	7.56E 04	3.64E 04	4.29E 04	2.30E 04	3.70E 04
374	182.04	4.31E 04	7.49E 04	3.61E 04	4.25E 04	2.28E 04	3.63E 04
376	186.52	4.27E 04	7.42E 04	3.58E 04	4.20E 04	2.26E 04	3.56E 04
378	191.08	4.23E 04	7.36E 04	3.55E 04	4.16E 04	2.25E 04	3.49E 04
380	195.73	4.19E 04	7.29E 04	3.51E 04	4.11E 04	2.23E 04	3.42E 04
382	200.47	4.14E 04	7.22E 04	3.48E 04	4.07E 04	2.21E 04	3.35E 04
384	205.29	4.10E 04	7.16E 04	3.45E 04	4.03E 04	2.19E 04	3.28E 04
386	210.21	4.06E 04	7.09E 04	3.42E 04	3.98E 04	2.18E 04	3.20E 04
388	215.22	4.02E 04	7.02E 04	3.39E 04	3.94E 04	2.16E 04	3.13E 04

TABLE 4; HENRYS LAW CONSTANT, ATM/MOLE FRACTION 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
390'	220.32	3.98E 04	6.95E 04	3.36E 04	3.90E 04	2.14E 04	3.05E 04
392	225.52	3.94E 04	6.89E 04	3.33E 04	3.86E 04	2.13E 04	2.97E 04
394	230.81	3.90E 04	6.82E 04	3.30E 04	3.82E 04	2.11E 04	2.89E 04
396	236.19	3.86E 04	6.76E 04	3.27E 04	3.78E 04	2.09E 04	2.81E 04
398	241.68	3.82E 04	6.69E 04	3.24E 04	3.74E 04	2.08E 04	2.72E 04
400	247.26	3.78E 04	6.63E 04	3.20E 04	3.70E 04	2.06E 04	2.64E 04
402	252.94	3.74E 04	6.56E 04	3.18E 04	3.66E 04	2.04E 04	2.55E 04
404	258.73	3.70E 04	6.50E 04	3.15E 04	3.62E 04	2.02E 04	2.45E 04
406	264.61	3.67E 04	6.43E 04	3.12E 04	3.59E 04	2.01E 04	2.36E 04
408	270.60	3.63E 04	6.37E 04	3.09E 04	3.55E 04	1.99E 04	2.25E 04
410	276.69	3.59E 04	6.30E 04	3.06E 04	3.51E 04	1.98E 04	2.14E 04
412	282.89	3.55E 04	6.24E 04	3.03E 04	3.48E 04	1.96E 04	2.01E 04
414	289.20	3.51E 04	6.18E 04	3.00E 04	3.44E 04	1.94E 04	1.86E 04
416	295.62	3.48E 04	6.11E 04	2.97E 04	3.41E 04	1.93E 04	1.64E 04
418	302.14	3.44E 04	6.05E 04	2.94E 04	3.37E 04	1.91E 04	
420	308.78	3.40E 04	5.99E 04	2.91E 04	3.34E 04	1.89E 04	
422	315.53	3.37E 04	5.92E 04	2.89E 04	3.30E 04	1.88E 04	
424	322.39	3.33E 04	5.86E 04	2.86E 04	3.27E 04	1.86E 04	
426	329.37	3.29E 04	5.80E 04	2.83E 04	3.24E 04	1.85E 04	
428	336.46	3.26E 04	5.74E 04	2.80E 04	3.20E 04	1.83E 04	
430	343.67	3.22E 04	5.68E 04	2.78E 04	3.17E 04	1.81E 04	
432	351.00	3.18E 04	5.62E 04	2.75E 04	3.14E 04	1.80E 04	
434	358.46	3.15E 04	5.55E 04	2.72E 04	3.11E 04	1.78E 04	
436	366.03	3.11E 04	5.49E 04	2.70E 04	3.08E 04	1.77E 04	
438	373.72	3.08E 04	5.43E 04	2.67E 04	3.05E 04	1.75E 04	
440	381.54	3.05E 04	5.37E 04	2.64E 04	3.02E 04	1.74E 04	
442	389.49	3.01E 04	5.31E 04	2.62E 04	2.99E 04	1.72E 04	
444	397.56	2.98E 04	5.26E 04	2.59E 04	2.96E 04	1.71E 04	
446	405.76	2.94E 04	5.20E 04	2.57E 04	2.93E 04	1.69E 04	
448	414.09	2.91E 04	5.14E 04	2.54E 04	2.90E 04	1.68E 04	
450	422.55	2.88E 04	5.08E 04	2.52E 04	2.87E 04	1.66E 04	
452	431.14	2.84E 04	5.02E 04	2.49E 04	2.84E 04	1.65E 04	
454	439.87	2.81E 04	4.96E 04	2.47E 04	2.82E 04	1.63E 04	
456	448.73	2.78E 04	4.91E 04	2.44E 04	2.79E 04	1.62E 04	
458	457.73	2.75E 04	4.85E 04	2.42E 04	2.76E 04	1.60E 04	
460	466.87	2.72E 04	4.79E 04	2.39E 04	2.73E 04	1.59E 04	
462	476.14	2.68E 04	4.73E 04	2.37E 04	2.71E 04	1.57E 04	
464	485.56	2.65E 04	4.68E 04	2.34E 04	2.68E 04	1.56E 04	
466	495.12	2.62E 04	4.62E 04	2.32E 04	2.66E 04	1.54E 04	
468	504.83	2.59E 04	4.57E 04	2.30E 04	2.63E 04	1.53E 04	
470	514.67	2.56E 04	4.51E 04	2.27E 04	2.61E 04	1.52E 04	
472	524.67	2.53E 04	4.46E 04	2.25E 04	2.58E 04	1.50E 04	
474	534.81	2.50E 04	4.40E 04	2.23E 04	2.56E 04	1.49E 04	
476	545.11	2.47E 04	4.35E 04	2.20E 04	2.53E 04	1.48E 04	
478	555.55	2.44E 04	4.29E 04	2.18E 04	2.51E 04	1.46E 04	

TABLE 4; HENRYS LAW CONSTANT, ATM/MOLE FRACTION 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
480	566.15	2.41E 04	4.24E 04	2.16E 04	2.49E 04	1.45E 04	
482	576.90	2.39E 04	4.19E 04	2.14E 04	2.46E 04	1.44E 04	
484	587.81	2.36E 04	4.13E 04	2.11E 04	2.44E 04	1.42E 04	
486	598.87	2.33E 04	4.08E 04	2.09E 04	2.42E 04	1.41E 04	
488	610.10	2.30E 04	4.03E 04	2.07E 04	2.39E 04	1.40E 04	
490	621.48	2.27E 04	3.98E 04	2.05E 04	2.37E 04	1.38E 04	
492	633.03	2.25E 04	3.93E 04	2.03E 04	2.35E 04	1.37E 04	
494	644.73	2.22E 04	3.87E 04	2.00E 04	2.33E 04	1.36E 04	
496	656.61	2.19E 04	3.82E 04	1.98E 04	2.31E 04	1.34E 04	
498	668.65	2.17E 04	3.77E 04	1.96E 04	2.29E 04	1.33E 04	
500	680.86	2.14E 04	3.72E 04	1.94E 04	2.27E 04	1.32E 04	
502	693.23	2.11E 04	3.67E 04	1.92E 04	2.25E 04	1.31E 04	
504	705.78	2.09E 04	3.62E 04	1.90E 04	2.23E 04	1.30E 04	
506	718.50	2.06E 04	3.57E 04	1.88E 04	2.21E 04	1.28E 04	
508	731.40	2.04E 04	3.52E 04	1.86E 04	2.19E 04	1,27E 04	
510	744.47	2.01E 04	3.47E 04	1.84E 04	2.17E 04	1.26E 04	
512	757.72	1.99E 04	3.43E 04	1.82E 04	2.15E 04	1.25E 04	
514	771.15	1.96E 04	3.38E 04	1.80E 04	2.13E 04	1.24E 04	
516	784.76	1.94E 04	3.33E 04	1.78E 04	2.11E 04	1.22E 04	
518	798.55	1.92E 04	3.28E 04	1.76E 04	2.09E 04	1.21E 04	
520	812.53	1.89E 04	3.24E 04	1.74E 04	2.07E 04	1.20E 04	
522	826.69	1.87E 04	3.19E 04	1.72E 04	2.05E 04	1.19E 04	
524	841.04	1.85E 04	3.14E 04	1.70E 04	2.04E 04	1.18E 04	
526	855.58	1.82E 04	3.10E 04	1.68E 04	2.02E 04	1.17E 04	
528	870.31	1.80E 04	3.05E 04	1.67E 04	2.00E 04	1.16E 04	
530	885.23	1.78E 04	3.00E 04	1.65E 04	1.98E 04	1.15E 04	
532	900.34	1.76E 04	2.96E 04	1.63E 04	1.97E 04	1.13E 04	
534	915.66	1.73E 04	2.91E 04	1.61E 04	1.95E 04	1.12E 04	
536	931.17	1.71E 04	2.87E 04	1.59E 04	1.93E 04	1.11E 04	
538	946.88	1.69E 04	2.83E 04	1.57E 04	1.91E 04	1.10E 04	
540	962.79	1.67E 04	2.78E 04	1.56E 04	1.90E 04	1.09E 04	
542	978.90	1.65E 04	2.74E 04	1.54E 04	1.88E 04	1.08E 04	
544	995.22	1.63E 04	2.69E 04	1.52E 04	1.87E 04	1.07E 04	
546	1011.75	1.61E 04	2.65E 04	1.50E 04	1.85E 04	1.06E 04	
548	1028.49	1.59E 04	2.61E 04	1.49E 04	1.83E 04	1.05E 04	
550	1045.43	1.57E 04	2.57E 04	1.47E 04	1.82E 04	1.04E 04	
552	1062.59	1.55E 04	2.52E 04	1.45E 04	1.80E 04	1.03E 04	
554	1079.96	1.53E 04	2.48E 04	1.44E 04	1.79E 04	1.02E 04	
556	1097.55	1.51E 04	2.44E 04	1.42E 04	1.77E 04	1.01E 04	
558	1115.36	1.49E 04	2.40E 04	1.40E 04	1.76E 04	1.00E 04	
560	1133.38	1.47E 04	2.36E 04	1.39E 04	1.74E 04	9.93E 03	
562	1151.63	1.45E 04	2.32E 04	1.37E 04	1.73E 04	9.83E 03	
564	1170.10	1.43E 04	2.28E 04	1.35E 04	1.72E 04	9.74E 03	
566	1188.80	1.42E 04	2.24E 04	1.34E 04	1.70E 04	9.65E 03	
568	1207.72	1.40E 04	2.20E 04	1.32E 04	1.69E 04	9.56E 03	

TABLE 4; HENRYS LAW CONSTANT, ATM/MOLE FRACTION 01/10/77 HEMA

DEGREES F	PSIA	OXYGEN	NITROGEN	HYDROGEN	HELIUM	XENON	METHANE
570	1226.88	1.38E 04	2.16E 04	1.31E 04	1.67E 04	9.47E 03	
572	1246.26	1.36E 04	2.12E 04	1.29E 04	1.66E 04	9.38E 03	
574	1265.89	1.34E 04	2.08E 04	1.27E 04	1.65E 04	9.29E 03	
576	1285.74	1.33E 04	2.04E 04	1.26E 04	1.63E 04	9.20E 03	
578	1305.84	1.31E 04	2.00E 04	1.24E 04	1.62E 04	9.11E 03	
580	1326.17	1.29E 04	1.96E 04	1.23E 04	1.61E 04	9.02E 03	
582	1346.75	1.28E 04	1.92E 04	1.21E 04	1.59E 04	8.94E 03	
584	1367.57	1.26E 04	1.88E 04	1.20E 04	1.58E 04	8.85E 03	
586	1388.64	1.24E 04	1.85E 04	1.18E 04	1.57E 04	8.77E 03	
588	1409.96	1.23E 04	1.81E 04	1.17E 04	1.56E 04	8.68E 03	
590	1431.52	1.21E 04	1.77E 04	1.16E 04	1.54E 04	8.60E 03	
592	1453.35	1.20E 04	1.73E 04	1.14E 04	1.53E 04	8.52E 03	
594	1475.42	1.18E 04	1.70E 04	1.13E 04	1.52E 04	8.44E 03	
596	1497.76	1.17E 04	1.66E 04	1.11E 04	1.51E 04	8.36E 03	
598	1520.36	1.15E 04	1.62E 04	1.10E 04	1.50E 04	8.28E 03	
600	1543.22	1.14E 04	1.59E 04	1.08E 04	1.48E 04	8.20E 03	