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Testing of the CONTAIN Code

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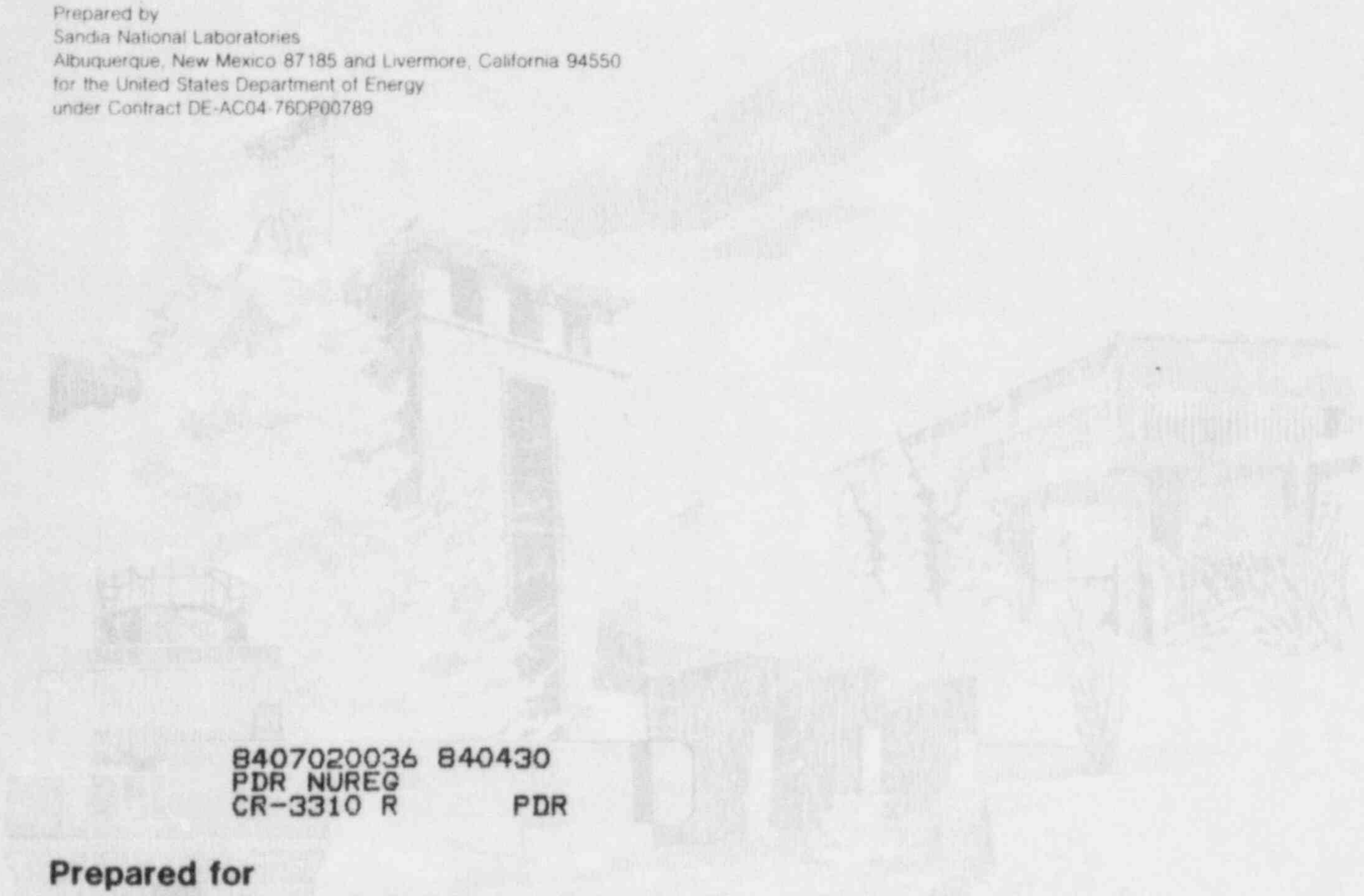

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TESTING OF THE CONTAIN CODE

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ABSTRACT

CONTAIN is a large computer code intended for use in the analysis of severe nuclear power plant accidents. Many tests have been conducted on CONTAIN to assess its adequacy for dealing with nuclear-accident problems. This report describes the CONTAIN test program and summarizes the results obtained to date. These results are presented so that users may be aware of the features of CONTAIN that have been checked and of the areas where problems have been identified. In addition, this report provides information needed by users to repeat tests of interest in their specific work areas.

The test efforts have identified a substantial number of problems in the coding or logic of the CONTAIN code. Most of these problems have been corrected. These corrections have been included in the most recent versions of the code. CONTAIN can accurately treat most of the phenomena expected to occur in containment atmospheres. Some problems identified by the test program, involving pool-related phenomena, have prompted the development of a substantially new system of models for pool phenomena. When completed, this new system will be subjected to intense testing of the type described here.

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1.0 INTRODUCTION

CONTAIN is a large computer code that has been designed to model the response of liquid-metal fast-breeder reactor (LMFBR) or light-water reactor (LWR) containments to severe accidents. The problems to which CONTAIN would normally be applied are generally highly complex and have a direct bearing on matters vital to nuclear plant safety. Because of its intended use in safety analyses, the CONTAIN code must, therefore, be thoroughly tested to ensure that the results generated by its use are credible.*

A program for testing the CONTAIN code has been established whereby various portions of the code can be methodically tested. Tests are designed to identify problems and errors that may exist in the various subroutines and modules of the code. Problem areas may simply consist of potential sources of confusion to the user, they may involve quantitative inaccuracies or logical errors that lead to invalid or inaccurate results, or they may entail conditions that actually prevent the code from running in certain modes.

The CONTAIN testing program has been underway for some time. Various of approaches have been utilized, all having the common goal of identifying problems or of establishing the credibility of the predictions of the code in one way or another. In much of the work done to date, specific test problems were selected that could be modeled using CONTAIN and that could be analytically solved by means of hand calculations. The CONTAIN results were then compared with the separate analytical results. If the two were in agreement, the CONTAIN results were presumed to be correct. If differences were evident, work was undertaken to identify the cause of the differences. Problems, inaccuracies, etc., attributed to CONTAIN were then flagged for correction.

Certain phenomena handled by CONTAIN are very complex and do not lend themselves to hand calculations. CONTAIN's results relative to these phenomena are checked using other codes that are in a more advanced state of development and that have been widely accepted. In some cases, such codes may not be available, so that quantitative checks on CONTAIN results are not always possible. As a minimum, however, a qualitative evaluation of the CONTAIN results is made.

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*The terms "verification" and "validation" are often used to describe procedures for establishing the credibility of a model. Because not everyone construes the meanings of these terms in similar ways, we hesitate to use them. Instead, we refer to the "testing" of the code and describe the different types and levels of testing that may be used to check the capabilities of the code. The word "validation" is used in some instances to indicate the corroboration of code predictions using experimental results.

The testing effort includes integrated test problems that exercise most of the options and modules in CONTAIN. These test problems are designed to simulate severe accident situations in LWRs and LMFBRs. Checks of CONTAIN's results for these integrated tests are made using whatever data or analyses are available for comparison. These integrated-problem results are also evaluated on a qualitative basis; that is, the overall results and trends predicted by CONTAIN are evaluated based on engineering judgement and experience.

Code validation efforts have also been initiated. In this work, CONTAIN results are compared with results derived from experiments. Two key areas have thus far been checked. The first involved the prediction of containment conditions following a blowdown from the primary system of a light-water reactor (LWR). The experiment was carried out in the HDR facility, a decommissioned LWR, in Germany. The second area of validation dealt with aerosol behavior. The aerosol behavior code validation and evaluation (ABCOVE) experiments conducted by Hanford Engineering Development Laboratories (HEDL) provided the actual data with which the code predictions were compared. Both of these validation efforts involved blind predictions, and in each case CONTAIN results were quite good[1]. These code validation efforts will be described in a separate report[2].

A list (not necessarily complete) of the features or capabilities of CONTAIN that require testing is presented below. Tests have been conducted and documented for each of these areas:

Two-Phase Atmosphere Thermodynamics (water vapor or sodium vapor in a noncondensible-gas atmosphere)
Source Tables
Intercell Gas Flow
Structure-to-Atmosphere Heat Transfer
Surface Condensation
Sodium-Spray Fire
Aerosol Transport in Intercell Gas Flow
Fission-Product Decay
Fission-Product Release and Acceptance
Fission-Product Intercell Transport
Fission-Product-Decay Heating
Hydrogen Combustion
Hydrogen Explosion
Sodium-Vapor Chemistry
Sodium-Pool Fires
Pool Chemical Reactions
Pool Heatup and Boiling
Pool-to-Atmosphere Heat Transfer
Restart Capability
Integrated LWR Capability

This report summarizes the results obtained to date in the CONTAIN test program. It presents these results so that users may be aware of the features of CONTAIN that have been checked and of the areas where problems have been identified. In addition, this report provides information needed by a user to repeat tests of interest in his specific work areas. The user may want to repeat certain tests, so that results obtained using his particular version of the code can be checked against documented test results.

A substantial number of tests have been completed. However, the test program represents an ongoing effort. I cannot be completed until the development of the code is completed. The current test effort represents the first phase in the overall testing program. Undoubtedly, several rounds of tests will be required before the program is completed. Additional testing will be necessary to check subsequent versions of the code as new models and modules are added to expand and improve the capabilities of existing versions.

Section 2 of this report describes the overall test program in more detail. The overall philosophy and each of the program elements are discussed. The actual test results are presented in Section 3. Test reports are presented, along with selected data sets, check calculations, or other means used to evaluate the capabilities and performance of the code. Section 4 discusses future test plans and presents a list of areas yet to be tested.

References:

1. K. K. Murata et al, "CONTAIN: Recent Highlights in Code Testing and Validation," in the Proceedings of the International Meeting on Light Water Reactor Severe Accident Evaluation, Aug. 28 to Sept. 1, 1983, (Stone and Webster Engineering Corp, 1983).

2. "Validation of the CONTAIN Code for Severe Reactor Accident Containment Analysis," to be published.

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2.0 TEST PROGRAM

An essential part of the development of a large computer code like CONTAIN is the testing of the code. A thorough test program entails many levels of testing, ranging from simple debugging to full-scale sensitivity analyses of the physical models on which the code is based. Such a program requires the efforts of many different people over a period of one or more years. Therefore, early in this program it was recognized that it would be desirable 1) to standardize testing procedures in order to prevent duplication of effort, and 2) to provide concurrent documentation of test efforts and test results so that this information would be readily available to the nuclear-safety research community.

No attempt has been made here to prescribe the extent of the testing needed to establish the credibility of CONTAIN as a predictive tool. It is unlikely that there will be a point at which it is decided that the test program is truly complete; there will always be some remaining uncertainties and new ideas about how to resolve the uncertainties. What is likely is that the testing process will be carried out like a series of successive approximations. For example, the initial efforts in this test program concentrated on tests of the treatment of single, isolated phenomena or on tests of single modules within CONTAIN. Testing has now progressed to the point where many complex interactions, occurring simultaneously, are being examined in some of the tests. As this testing process is continued, confidence in the code will grow, and there will likely be a continuous increase in the extent to which the code is used in reactor-safety research applications.

Because of the complexity of the code, it was essential that the test program be well organized from the beginning and that adequate documentation be maintained and available throughout the testing effort. Given these features of the program, it would then be possible to review the overall status of CONTAIN testing at any given time in order to decide what should be done next, i.e., to determine priorities for testing based on the most current technical and programmatic information. In addition, it would be possible to check, quickly and easily, the performance of revised versions of the code using test problems that had run successfully in previous versions. It would also be possible to provide concise documentation about each test to all users in order to allow them to form their own opinions about the applicability of the code to the analysis of their particular problems. The standardized procedures described in the next sections were developed in pursuit of these goals.

The following discussions present the overall approach and guidelines established for the CONTAIN test program. General policies are discussed, and formats for specific documents are given. It is expected that these guidelines will be modified as practical problems are encountered or as better ideas are generated.

2.1 TYPES OF TESTS

2.1.1 Software vs. Physics Tests

There are several ways to characterize the tests that need to be performed on a code such as CONTAIN. For example, there are tests of software (coding) and tests of the physical models that are the basis of the software. Most tests of CONTAIN necessarily test both physics and coding simultaneously, but because the goal is to achieve maximum accuracy and reliability in the predictions of the code, the adequacy of the modeling of the physics is the primary focus of the tests. The choice of physical parameters used in the models is also a critical issue. This issue may merit separate consideration and assessment, especially near the end of the code-development process.

2.1.2 Module vs. Integrated Tests

Tests may be characterized as module tests or integrated tests. The distinction is important because the results of module, or "single-effect," tests are more amenable to detailed quantitative comparison with the results of exact analytic calculations or with results obtained using established, highly reliable computer codes. Integrated tests, on the other hand, do not usually lend themselves to direct quantitative comparisons with other calculations, because the mathematics required is too complex for hand calculations and because there are no existing codes that can model all the phenomena treated by CONTAIN. Thus, for integrated tests, the emphasis must be placed on checking for internal consistency, checking conserved quantities, and when feasible, making comparisons with experiments.

2.1.3 Parameter Sensitivity

Ideally, complete testing of a large physics code requires that all tests be performed over the entire conceivable range of relevant physical parameters. These parameters would include not only input parameters, but also any parameters that might be altered internally (e.g., material properties). The complexity of the test effort required to do this is staggering. Such complete testing is probably not possible, nor is it practical. Nonetheless, in some cases it is important to investigate the domain of the parameter space over which CONTAIN is expected to be accurate. It may sometimes be more important to test for error sensitivity of some critical parameter than to proceed with a higher-level test (see Subsection 2.2.2).

When a sensitivity test should be done is a matter of judgment. Because it is impractical to explore sensitivities over the entire N-dimensional parameter space, physical intuition may be the most important factor in guiding the tester to those parts of the parameter space that might cause problems in CONTAIN.

2.2 STANDARDIZED TEST PROCEDURES

2.2.1 Testing Guidelines

Guidelines have been established for carrying out the CONTAIN test program. The following guidelines are not applicable in all situations, and therefore they should be used judiciously.

1. The test problem should be conceived in detail before it is run on the computer. It is, however, probably prudent to run the problem on CONTAIN before committing large amounts of time on detailed hand calculations, because the test problem may not run as originally conceived. It is also essential to resist the temptation to use the code listing, the code manual, or the code output to learn how the calculation "should" be done, because this could easily result in a failure to detect flaws in the original coding.

2. The tester should not be the module developer. It is very easy for the person who developed a module to overlook ways in which it might be made to give incorrect results. The developer's assistance in setting up the problem may be desirable, but the test problem itself should be conceived independently. Although test problems devised and used during program development are of interest--and their input data sets may be filed with the other input files--they should not be used in the CONTAIN testing program.

3. In assessing the results of tests, quantitative comparisons should be made using reference quantities that can be directly compared with the CONTAIN output variables. Manipulation of the CONTAIN output variables to obtain derived quantities, which can then be used for comparison with, for example, handbook values, is an unsatisfactory approach because such manipulation may entail tacit assumptions (e.g., the form of the equation of state) not appropriate to the code. Instead, the handbook values should be converted to numbers that can be compared with the CONTAIN printout. This approach also allows subsequent versions of CONTAIN to be tested against the same numbers. (For some types of consistency checks, this will not be possible, but every attempt should be made to make checkouts of future code versions as simple as possible.)

4. All tests should be run without the use of modifications to the code. It is intended that subsequent versions of the code be tested using data sets from the original tests. If code modifications are used in the initial testing, this may make testing of later versions difficult. (If the built-in code debugging and diagnostic capabilities are not adequate for use in tests of the module or modules of interest, a permanent change in the debugging/diagnostic capabilities should be made and included in the next version of CONTAIN.)

5. The goal of testing is to identify problems, not to correct them. Therefore, a test report should not be delayed because a problem is likely to be corrected in an imminent version of the code.

2.2.2 Levels of Testing

Several terms have been defined to characterize tests by the level of detail involved. These terms are useful in keeping track of the progress made in the overall testing program. The test levels (TL) are:

TL1 - A functional test to determine whether or not the code runs without crashing

TL2 - A qualitative test to determine whether or not the results are physically reasonable

TL3 - A consistency test to demonstrate that conserved quantities are in fact conserved or that test results are insensitive to certain parameters as they should be

TL4 - A quantitative test that involves detailed comparison of the output with the results of another calculation--either the results from an exact analytic calculation (TL4A) or the results from another computer code (TL4C), the credibility of which is well established

TL5 - An experiment-based test that entails comparison with experimental results when all of the relevant features of the experiment are capable of being modeled by CONTAIN

2.2.3 Standard Test Set and Spot Checks

As new versions of the code are developed, it is important to verify that no capabilities of previous versions have been lost. However, it would be excessively time-consuming to rerun all the tests. Therefore, for each test series, one or two "standard" tests should be selected that can be run, as a routine quality-control procedure, on all major new versions. For each of the standard tests, a simple "spot check" should be specified. The purpose of the spot check is to verify that the new version produces the same output as the older, thoroughly tested version. The simplest way to do this is to copy a page from the output of the tested version and to circle two or more numbers with which the output of the new version can then be compared. The numbers chosen for the spot checks should be carefully selected, because it might be possible for a new version to reproduce some parts of the calculation but not others.

2.2.4 Documentation

Information on CONTAIN tests is stored in computer files and in hard-copy files. Each test is identified by a number consisting of two letters that define the test series plus two digits that define the specific test in the series. (For example, HS03 indicates the third test in a series designed to test the treatment of heat transfer to structures.) In general, the first two letters have been mnemonically related to the subject of the test -- AC for atmosphere condensation, FP for fission products, etc. Standard tests are identified by (ST) appended to the ID number, e.g., BB06(ST).

2.2.4.1 Test Summary Report

This is a short, preferably one-page, summary of all relevant information on one or more tests in a test series. Each Test Summary Report is generated and stored on the computer. The computer file containing all such reports comprises the base file from which several other files obtain information.

The format used in each Test Summary Report is as follows:

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: USER NAME:
2. TEST LEVEL:
3. TITLE OF TEST:
4. CODE VERSION (DATE OF TEST):
5. ACTIVE MODULES OR OPTIONS:
6. CONTAINMENT CONFIGURATION AND SOURCES:
7. TEST:
8. RESULTS OF TEST:
9. COMMENTS:
10. SUGGESTIONS FOR ADDITIONAL TESTS:

The code version given in Item 4 of each Test Summary Report indicates by a three-character alphanumeric group the creation date of the particular version of CONTAIN used in that test. For example, code version 208 was created on February 8 (1982), code version 312 on March 12 (1982), and so on. The letters A, B, or C in the first position of the code version designation refers to October, November, or December, respectively. The successive code versions correspond to the progressive development of CONTAIN. The different versions referred to in this report include, in the order of their creation dates: 208, 308, 312, 501, 809, 915, A20 (all created in 1982), 120, and 705 (both created in 1983).

2.2.4.2 Problem Report

Very brief descriptions of any bugs or other problems are included in each Test Summary Report (between the ======== lines). A problem is reported whether or not it has been or is being fixed. Each problem is given an identification number consisting of the test identification number plus two digits. (For example, problem number AA03-01 is the first problem identified in test AA03.) Reportable problems include potential sources of confusion to the user as well as serious errors.

The format for the Problem Report is as follows:

```
==================================================================
1.  PROBLEM:  ID NO.          2.  LEVEL:  PL          3.  RESOLVED?
4.  DESCRIPTION:
5.  DATE PROBLEM RESOLVED:
==================================================================
```

Four problem levels (PLs), which can be used to establish priorities for corrective action, have been defined. The PLs are:

PL1 - An inconvenience or potential source of confusion to the user. No errors are generated, however, if input and output are properly understood;

PL2 - Relatively small quantitative errors occur. These errors may be acceptable in some applications and/or parameter regimes, but are unacceptable in other applications or for untested parameter choices;

PL3 - Large quantitative errors occur for many parameter choices of interest--a major quantitative bug (actually more dangerous than PL4);

PL4 - The problem will not run. The code aborts or "bombs".

2.2.4.3 Input Data Set

The data file used for each test run should be made available to other users. This is essential if future versions of the code are to be run using previously developed test problems. Consequently, Input Data Sets are stored on a computer file that is accessible to other users. Each Input Data Set should have the test ID number on the first title card, and if the test is a standard test, this fact should also be indicated on the title card. Comments that will aid other users in understanding the input should be provided at appropriate locations within the Input Data Set.

2.2.4.4 Hard-Copy File

Each test series, when complete, has a folder containing the following:

1. A copy of the Test Summary Report and the Input Data Set;
2. Supporting calculations and comparisons (generally handwritten). These should be in sufficient detail to allow the reader to follow the analysis without consulting the tester;
3. Test output, including plots, on microfiche;
4. For standard tests only, a sheet defining the spot checks. This sheet identifies key output numbers that are used in verifying that new versions of the code produce essentially the same results as previous versions.

2.2.4.5 Status Chart and Index

The Status Chart is a computer file that shows the state of progress in testing each feature of the code, including the levels of tests performed and the relevant test identification numbers. The Index is a file containing entries that consist of the first two lines of each Test Summary Report.

BIBLIOGRAPHY:

1. Myers, G. J. *Software Reliability*. New York: Wiley Interscience, 1976.
2. Senglaub, M. E. CNTNPLT Input Description. RS4450/882/32.
3. Tausworthe, R. C. *Standardized Development of Computer Software*. Englewood Cliffs, NJ: Prentice-Hall, 1979.
4. Yourdon, E. *Techniques of Program Structure and Design*. Englewood Cliffs, NJ: Prentice-Hall, 1975.

3.0 TEST PROGRAM RESULTS — TEST REPORTS AND ANALYSIS

This section presents the results achieved to date in the CONTAIN test program. The Test Summary Reports are provided, along with brief discussions of the supporting analyses used to check the code outputs. The Input Data Sets used in making the "standard test" runs are also provided. Input Data Sets used in tests other than the standard tests are included on microfiche with each copy of this report. Thus, the information presented shows what areas or features have been tested, shows the results of the tests, and includes information so that other users can rerun the tests on their versions of CONTAIN and carry out similar supporting analyses.

Test Summary Reports are grouped together in test areas according to the types of phenomena being modeled. For example, the first group includes tests that deal with atmosphere thermodynamics and heat transfer; the second group includes tests that deal with atmosphere chemical reactions. There is some unavoidable overlap among these groups, but each grouping is used to emphasize certain features or capabilities of the code.

Table 3-1 shows the organization of the tests presented in this section. The general test area is indicated, together with the various test series included in that area. The test-series identification letters are also shown.

Table 3-1 Organization of test reports

- 3.1 Atmosphere-Thermodynamics and Heat-Transfer Tests
    - 3.1.1 Series AA - Atmosphere Thermodynamics with Sources
    - 3.1.2 Series AC - Condensation Heat Transfer to Structures
    - 3.1.3 Series HS - Transient Heat Conduction in Structures
    - 3.1.4 Series VA - Sodium- and Water-Vapor Thermodynamics
- 3.2 Atmosphere-Chemistry Tests
    - 3.2.1 Series HB - Hydrogen Burns
    - 3.2.2 Series SB - Sodium-Vapor Combustion and Na_2O/H_2O Reactions
    - 3.2.3 Series SF - Sodium-Spray Fires
- 3.3 Intercell-Flow Tests
    - 3.3.1 Series CF - Intercell Flow of Gases
    - 3.3.2 Series AF - Intercell Flow of Aerosols
- 3.4 Fission-Product Tests
    - 3.4.1 Series FP - Fission-Product Decay and Release

Table 3-1 (Continued)

3.4.2 Series FT - Fission-Product Intercell Transport
3.4.3 Series FH - Fission-Product Heating of Structures

3.5 Pool-Thermodynamics and Heat-Transfer Tests

3.5.1 Series PQ - Pool-to-Atmosphere Heat Transfer
3.5.2 Series PB - Pool Heatup and Boiling
3.5.3 Series PS - Pool Sources
3.5.4 Series PC - Pool Chemistry
3.5.5 Series PF - Sodium-Pool Fires

3.6 Aerosol-Behavior Tests

Series AB - Aerosol Behavior

3.7 Integrated LWR Sample Problem

Series ZT - LWR Sample Problem

Each test series in each test area is introduced with explanatory comments. Test Summary Reports for each test series follow these comments. These reports are in the format discussed in Section 2. In some cases, the reports have been expanded to include figures or plots that enhance the understanding of the code results. Each Test Summary Report is followed by the Problem Reports, if such reports are needed. The supporting analysis used to check the CONTAIN results is presented next. This is followed by the Input Data Set(s) for the standard test(s) in each test series. Thus, the ordering of the information for each test series is as follows:

1. Introductory comments
2. Test reports, including figures where appropriate
3. Problem reports
4. Supporting analysis
5. Input data set(s) for the standard test(s) in the test series

In certain test series, no individual tests have been designated as standard, and therefore no input data sets are provided. In those sets that are provided, the machine-control input, which identifies the type of computer and the type of data storage to be used, has not been included at the beginning of these data sets, because this mandatory input is machine-dependent and will need to be specified accordingly.

Various problems were identified in a majority of the test areas. These problems were usually identified in the early tests of each test series. As testing proceded, corrections or improvements to the CONTAIN modeling were also identified. These corrections were tested using coding updates and were incorporated into subsequent versions of the code. The later (more recent) tests in each test series were performed, in some instances, after improvements to the code had been made. Thus, the later tests in each series best reflect the current status of CONTAIN.

3.1 ATMOSPHERE-THERMODYNAMICS AND HEAT-TRANSFER TESTS

3.1.1 Series AA - Atmosphere Thermodynamics with Sources

This series of tests was carried out to check the performance of the atmosphere thermodynamics models in CONTAIN. In particular, these tests dealt with the thermodynamics of water vapor and noncondensible gas mixtures. Water vapor was introduced into a cell filled with air. The source routines and options in CONTAIN were also checked out.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: AA01(ST), AA02, AND AA03 USER NAME: K. D. BERGERON

2. TEST LEVEL: TL4A

3. TITLE OF TEST: ATMOSPHERE THERMODYNAMICS WITH SOURCES

4. CODE VERSION (DATE): 208 (2/16/82); 312 (3/31/82)

5. ACTIVE MODULES OR OPTIONS: FLOWS, THERMAL. HEAT TRANSFER IS OFF.

6. CONTAINMENT CONFIGURATION AND SOURCES: ONE CELL INITIALLY AT ONE ATMOSPHERE AND 294 K. STEAM/WATER MIXTURE INJECTED VIA MASS AND ENTHALPY TABLES OVER A 23 S PERIOD. PRESSURE SHOULD RISE TO A CONSTANT VALUE AFTER 23 S (ADIABATIC WALLS).

7. TEST: (1) COMPARE TOTAL MASS AND ENTHALPY IN FINAL STATE WITH HAND-INTEGRATION OF SOURCE TABLES. (2) COMPARE FINAL PRESSURE AND TEMPERATURE WITH VALUE OBTAINED BY HAND CALCULATION FROM STEAM TABLES. PRESSURE RISE OF AIR DUE TO HEATING MUST BE INCLUDED IN CALCULATION.

8. RESULTS OF TEST: (1) TOTAL MASS AND ENTHALPY IN EXACT AGREEMENT WITH INTEGRATION OF SOURCE TABLE.
   (2) FINAL PRESSURE AND TEMPERATURE WITHIN 4% AND .4%, RESPECTIVELY, OF STEAM TABLE CALCULATION. (NOTE HAND CALCULATION DID NOT ACCOUNT FOR ENTHALPY INCREASE DUE TO HEATING OF THE AIR, WHICH MAY ACCOUNT FOR PART OF THE DISCREPANCY.)
   (3) QUALITATIVE BEHAVIOR IS EXACTLY AS EXPECTED: PRESSURE REACHES A PLATEAU AT EXACTLY THE END OF THE BLOWDOWN, AND HOLDS CONSTANT INDEFINITELY THEREAFTER.

9. COMMENTS: TEST AA02 GAVE SIMILAR RESULTS WITH A SYSTEM TIME STEP OF 20 S, WHICH IS ESSENTIALLY THE ENTIRE BLOWDOWN TIME. THESE TWO REPRESENT A FAIRLY RIGOROUS TEST OF ATMOSPHERE THERMODYNAMICS FOR WATER. TEST AA03 USED THE IFLAG=1 OPTION ON THE SOURCE TABLES, WHICH ASSUMES CONSTANT (NOT INTERPOLATED) VALUES BETWEEN SUCCESSIVE TABLE ENTRIES. FINAL H2O MASS AND ENERGY WERE, AGAIN, IN EXACT AGREEMENT WITH HAND INTEGRATION OF SOURCE TABLE DATA.

10. SUGGESTIONS FOR ADDITIONAL TESTS: SAME TEST WITH SODIUM COOLANT.

==

1. PROBLEM: ID NO.AA01-01 2. LEVEL: PL1 3. RESOLVED? YES

4. DESCRIPTION: INPUT INSTRUCTIONS SHOULD MAKE IT CLEAR THAT THE UNITS OF THE ENTHALPY SOURCE TABLE ARE J/KG, NOT WATTS.

5. DATE PROBLEM RESOLVED: 3/10/82

==

==

1. PROBLEM: ID NO.AA01-02 2. LEVEL: PL2,3 3. RESOLVED? YES

4. DESCRIPTION: ATMOSPHERE DENSITY PRINTED IN LONG EDIT INCLUDES MASS OF LIQUID-WATER FRACTION OF H2OV. IT SHOULD ONLY INCLUDE VAPOR FRACTION. THIS HAS CAUSED A PROBLEM IN THE CONTAINMENT SPRAY MODEL WHEN THIS QUANTITY WAS USED FOR DESCRIBING BEHAVIOR OF THE FALLING SPRAY DROPLET.

5. DATE PROBLEM RESOLVED: 4/83

==

Supporting Analysis: AA Series - Atmosphere Thermodynamics with Sources

Source-Table Check

The source table test is straightforward. With the IFLAG=2 option, the source table is interpolated between points. Therefore, a hand integration can be done using a trapezoidal rule. This can be done for both mass and energy, and compared with the atmosphere printout after the blowdown is over (no energy is lost since heat transfer is turned off). Results are shown in Table 3-2.

Table 3-2 Source table check

Quantity	Hand Calc.	CONTAIN
CONTAIN AA01 (IFLAG=2)		
Mass (kg)	2.03E5	2.04E5
Enthalpy (J)	2.26E11	2.23E11
CONTAIN AA03 (IFLAG=1)		
Mass	2.372E5	2.378E5
Enthalpy	2.63E11	2.63E11

Thermodynamics Check

Since heat transfer from the atmosphere is turned off, the final pressure and temperature can be calculated by means of the steam tables. What is known is total H_2O mass, total noncondensible mass, and total internal energy (initial internal energy plus enthalpy in the blowdown). To simplify the hand calculation, we neglect the heat capacity of the noncondensible gas, so its enthalpy is the same before and after the blowdown. The internal energy of the water is therefore just the total blowdown enthalpy divided by the total blowdown mass, which is U = 1113 kJ/kg. The specific volume is V = .292 m^3/kg. Unfortunately, these two thermodynamic functions are not commonly provided in steam tables. We must work, therefore, with enthalpy, H, and use

$$U_{fg} = H_{fg} - PV_g \tag{3.1-1}$$

$$U_f = H_f \tag{3.1-2}$$

$$X = (1113. - H_f)/U_{fg} \tag{3.1-3}$$

$$V_{mix} = XV_g \tag{3.1-4}$$

where

$U_{fg} = U_g - U_f$ = internal energy of vaporization of condensible material

$H_{fg} = H_g - H_f$ = enthalpy of vaporization of condensible material

P = pressure

V_g = specific volume of vapor

X = quality of steam = ratio of vapor mass to total mass of condensible material

V_{mix} = specific volume of vapor/liquid mixture

This sequence of calculations allows us to calculate V_{mix} for each pressure entry in the steam tables (which provides H_{fg} and V_g). We find $V_{mix} = .2989$ for $P = .18$ MPa, and $V_{mix} = .2663$ for $P = .20$ MPa. Interpolating, we find the value of P at which $V_{mix} = .292$ to be $P = .1842$ MPa. The interpolated temperature is 390.8 K. To this we add the noncondensible pressure

$$P_{nc} = \frac{T_{final}}{T_{initial}} P_{initial} \tag{3.1-5}$$

The final hand calculation is, therefore,

$$P_{tot} = 3.174E5 \text{ Pa} \qquad T = 390.8 \text{ K}$$

The CONTAIN prediction is

$$P_{tot} = 3.042E5 \text{ Pa} \qquad T = 389.3 \text{ K}$$

These differ by 4% and 0.4%, respectively.

This level of agreement is probably adequate verification of the code calculations, considering the simplifications made in the hand calculations. To check the model more carefully, a computer program written for the MEDICI code was used after the test report was completed. This program performed the iterative calculations required when simplifying assumptions are not made. An additional type of check is to use the value of steam quality printed in the code output to calculate pressure directly from the sources and the steam tables. Both types of tests gave much better agreement than the hand calculations; they showed CONTAIN to be correct within 1 degree in temperature and 2% in total pressure.

SERIES AA STANDARD TEST INPUT DATA SET

```
        && CONTAIN TEST IDENT AA01(ST) --- ATMOSPHERE THERMODYNAMICS

CONTROL = 9 1 2 1 2 1 0 0 0 0
MATERIAL
COMPOUND N2 O2 H2OL H2OV CONC FE
FISSION DUM1 DUM2
TIMES 59. 0. 1. 5. 40. 1.
FISSION
0 2
DUM1 DUM2
1.0E8 1.0E10
2*2.5E4 EOI
TITLE
CONTAIN TEST IDENT AA01(ST)
ATMOSPHERE THERMODYNAMICS WITH SOURCES -- 2/10/82

THERMAL
FLOWS
PRHEAT
PRFLOW


CELL=1
CONTROL = 18 0 0 7 6
  0 0 1 14 0
  0 0 0 0 0 0
  0 0 0

GEOMETRY 5.95E4, 48.03

HT-TRAN OFF OFF OFF OFF OFF OFF OFF
         && ......................ADIABATIC ATMOSPHERE....

STRUC

  R1,ROOF,SPHERE,6,0,300.
  19.85,0.,300.
  19.85,19.855,19.87,19.88,20.13,20.39,20.64
  FE,FE,FE,CONC,CONC,CONC

  F1,FLOOR,SLAB,4,0,300.
  19.85,0.,300.,1.24E3
  0.,.005,1.33,2.67,4.
  CONC,CONC,CONC,CONC

  W1,WALL,CYLINDER,6,0,300.
  38.1,0.,300.,38.1
  19.85,19.855,19.87,19.88,20.24,20.6,20.95
  FE,FE,FE,CONC,CONC,CONC
```

```
  W2,WALL,CYLINDER,6,0,300.
   38.1,0.,300.,38.1
   19.85,19.855,19.87,19.88,20.24,20.6,20.95
   FE,FE,FE,CONC,CONC,CONC

  SINK1,WALL,SLAB,3,1,300.
   10.,0.,1.41E4
   0.,.005,.300,.305
   CONC,CONC,CONC

  SINK2,WALL,SLAB,3,1,300.
   10.,0.,1.4E3
   0.,.001,.00535,6.35E-2
   FE,FE,FE

  SINK3,WALL,SLAB,3,1,300.
   10.,0.,1.61E5
   0.,.001,.003,3.81E-3
   FE,FE,FE


 ATMOS=3
 1.003E5 294.2
 N2=.795 O2=.195 H2OV=-1.E-5 && ESSENTIALLY DRY INITIAL ATMOSPHERE


 SOURCE=1
   H2OV=14
   IFLAG=2
    T=  0.     0.2    0.7    1.2    2.2    3.2    4.2    8.2    10.2
  15.2   20.2   22.7   23.2   1000.

MASS= 0.691E4 2.971E4 2.717E4 2.457E4 1.964E4 1.693E4 1.516E4
      0.965E4 0.827E4 0.381E4 0.216E4 0.011E4 0. 0.

 ENTH= 1.131E6 1.126E6 1.127E6 1.131E6 1.117E6 1.113E6 1.108E6
       1.142E6 1.138E6 1.102E6 0.629E6 0.454E6 0. 0.
 EOI
 EOF
```

3.1.2 Series AC - Condensation Heat Transfer to Structures

As indicated by the title, this test series dealt with condensation heat transfer to structures. Some of the tests used mixtures of condensible with noncondensible gases. Other tests used pure vapors. Different types of structures (heat sinks) were employed, and the effect of their orientation (roofs, walls, floors) on the extent of heat transfer was checked.

This test series resulted in the identification of a number of problems which led to the development of a major reformulation of the model for condensation on structures. Since this series represents one of the major successes of the test program (success being defined somewhat paradoxically as identification of problems), it is of interest to reproduce the test reports which relate to the old version of the model and to the problems identified before the new model was implemented. These are the reports numbered AC0X, which are to be distinguished from tests which use the new version, numbered AC2X.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: AC01-AC03, AC05, AC07 USER NAME: K. D. BERGERON

2. TEST LEVEL: TL4A

3. TITLE OF TEST: CONDENSATION ON STRUCTURES

4. CODE VERSION (DATE): 312 (3/16/82)

5. ACTIVE MODULES OR OPTIONS: FLOWS, CONDENSE, ATMOSPHERE SOURCES.

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE, LARGE CELL (RCB SIZE) WITH BLOWDOWN OF STEAM DURING FIRST 23 S (LIKE AA01), AND WITH CONDENSE TURNED ON. SEVERAL HEAT TRANSFER STRUCTURES TO ANALYZE, BOTH AS BOUNDARY STRUCTURES AND AS INTERIOR STRUCTURES. A CONCRETE HEAT SINK (SINK1) WAS THE PRIMARY FOCUS OF ATTENTION, BECAUSE THE THERMAL PROPERTIES OF CONCRETE USED IN CONTAIN ARE TEMPERATURE INDEPENDENT.

7. TEST: CALCULATE EFFECTIVE CONDENSATION HEAT TRANSFER COEFFICIENTS. TEST FOR ZONING AND TIME-STEP SENSITIVITY. ATTEMPT COMPARISON WITH PUBLISHED RESULTS.

8. RESULTS OF TEST: THE CONDENSE OPTION SEEMED TO FUNCTION PROPERLY. FOR EXAMPLE, H2OL BEGAN TO APPEAR IN THE CELL PRINTOUT (THIS WAS THE LIQUID COLLECTING ON THE ROOF ONLY). A FORMULA WHICH CALCULATES THE ATMOSPHERE-STRUCTURE HEAT TRANSFER COEFFICIENT (HTC) BY LOOKING AT NODE TEMPERATURES AT DIFFERENT TIME STEPS WAS DERIVED AND PROGRAMMED ON A CALCULATOR. TO TEST THE PROGRAM, CONDENSE WAS TURNED OFF IN RUN AC07, SO THE HTC SHOULD BE THE CONSTANT CONVECTIVE VALUE, HAS = 6.08, WHICH IT WAS. THE VALUE OF THE HTC FOR CONDENSATION ON WALLS WAS FOUND TO BE 14.4, WHICH SEEMS LOW. EXPERIMENTS (TAGAMI-UCHIDA, REFS 1 & 2) INDICATE THAT VALUES MORE LIKE 200 TO 300 WOULD BE MORE APPROPRIATE.

(ADDENDUM--8/11/82. THE LARGE DIFFERENCE BETWEEN THE CALCULATED AND EXPECTED HTC WAS FOUND TO BE DUE TO A NUMBER OF CODING ERRORS IN THE CONDENSATION MODEL AND IN THE PRSATX ROUTINE. THESE CORRECTIONS HAVE BEEN INCORPORATED IN VERSIONS 501 AND BEYOND. NEW CONDENSATION RESULTS ARE NOW IN BETTER AGREEMENT WITH TAGAMI-UCHIDA, THOUGH STILL LOW BY ABOUT A FACTOR OF 3. A COMPLETELY NEW CONDENSATION ROUTINE IS BEING DEVELOPED, WHICH WILL GIVE BETTER RESULTS AND ALSO RESOLVE SOME OF THE OTHER PROBLEMS IDENTIFIED IN THIS TEST SERIES.)

TESTS AC02, AC03, AND AC05 TESTED ZONING AND TIME-STEP SENSITIVITY. COARSE ZONING (AC02) RESULTED IN A DRAMATIC INCREASE IN THE HTC TO 211. FINER ZONING (AC03) HAD ONLY A 10% EFFECT. THIS TREND WAS UNDERSTANDABLE BECAUSE THE DIFFUSION LENGTH ASSOCIATED WITH THE TIME USED FOR THE CALCULATIONS (25 S) WAS 5 CM; THE FIRST ZONES OF TESTS AC01, AC02, AND AC03 WERE, RESPECTIVELY, .5 CM, 15 CM, AND .2 CM. WE CONCLUDE THAT ZONING SENSITIVITY WILL APPEAR WHEN THE FIRST ZONE SIZE IS GREATER THAN OR OF THE ORDER OF THE DIFFUSION LENGTH (GIVEN BY SQRT(4AT), WHERE A IS THE THERMAL DIFFUSIVITY) FOR THE TIMES, T, OF INTEREST.

9. <u>COMMENTS</u>: FUNCTIONALLY, THE CONDENSATION ROUTINE WORKS WELL, AND THE GENERAL TREND OF THE THERMAL BEHAVIOR IS AS EXPECTED, BUT THERE ARE SEVERAL QUESTIONS ABOUT QUANTITATIVE ACCURACY, WHICH NEEDS FURTHER ANALYSIS.

10. <u>SUGGESTIONS FOR ADDITIONAL TESTS</u>: TESTS AGAINST EXPERIMENTAL RESULTS, E.G., CAROLINA-VIRGINIA TUBE REACTOR EXPERIMENTS. ALSO, A COMPARISON AGAINST A GOOD BLOWDOWN CODE, E.G. CONTEMPT. MORE ANALYSIS IS DEFINITELY NEEDED.

===

1. PROBLEM: ID NO.AC01-02 2. LEVEL: PL3 3. RESOLVED? YES
4. DESCRIPTION: CONDENSATION HEAT TRANSFER RATES PREDICTED BY CONTAIN ARE SMALLER BY A FACTOR OF 70 THAN TAGAMI-UCHIDA CORRELATIONS
5. DATE PROBLEM RESOLVED: APRIL, 1982. CODING ERRORS CORRECTED. NEW RESULTS ARE OF SAME ORDER AS TAGAMI-UCHIDA, THOUGH STILL SOMEWHAT LOW. ADDENDUM 4/4/83. THE NEW CONDENSATION MODEL IS WITHIN 63% OF UCHIDA CORRELATIONS.

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1. PROBLEM: ID NO.AC01-3 2. LEVEL: PL2,3 3. RESOLVED? YES
4. DESCRIPTION: EVAPORATION FROM STRUCTURE SURFACES AND POOL ARE NOT MODELED IN CONTAIN. THIS CAN CAUSE THE ATMOSPHERE TO SUPERHEAT ARTIFICIALLY. THE NEW CONDENSATION MODEL WILL CORRECT THIS DEFICIENCY.
5. DATE PROBLEM RESOLVED: 9/30/82--NEW CONDENSATION MODEL; SEE AC22.

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CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: AC06 USER NAME: K. D. BERGERON

2. TEST LEVEL: TL4A

3. TITLE OF TEST: STRUCTURE CONDENSATION: PURE VAPOR

4. CODE VERSION (DATE): 312 (3/16/82); 120 (4/13/83)

5. ACTIVE MODULES OR OPTIONS: SAME AS AC01

6. CONTAINMENT CONFIGURATION AND SOURCES: SAME AS AC01, BUT INITIAL AIR IN CELL IS REPLACED WITH H2O TO GIVE A PURE VAPOR. (ACTUALLY A SMALL QUANTITY--1 PART IN 1,000--OF AIR REMAINS TO KEEP CODE INPUT AS IDENTICAL AS POSSIBLE.) INITIAL PRESSURE (AND MASS OF VAPOR) IS CONSIDERABLY LESS, SO THAT THE INITIAL TEMPERATURE CAN BE ABOUT THE SAME AS AC01.

7. TEST: CALCULATE HEAT TRANSFER COEFFICIENT (HTC) AND COMPARE WITH FORMULAS FROM BIRD, STEWART AND LIGHTFOOT (REF 3, EQ. 13.6-6) FOR PURE VAPOR CONDENSATION HTC ON VERTICAL WALLS AND NATURAL, TURBULENT CONVECTION.

8. RESULTS OF TEST: BSL PREDICTS 2.E4 FOR THE HTC. CONTAIN GIVES 15.7, ONLY SLIGHTLY LARGER THAN THE CASE WITH 1 ATM OF NONCONDENSIBLE GAS (AC01). THIS IS A DISCREPANCY OF THREE ORDERS OF MAGNITUDE.

9. COMMENTS: TO BE FAIR, THE MODEL DOES NOT TRY TO TREAT THE PURE VAPOR CASE, IN WHICH KINETIC EFFECTS, NOT BINARY DIFFUSION, ARE THE RATE-LIMITING PROCESSES. THE POINT IS THAT ONE SHOULD NEVER USE THIS MODEL FOR CASES IN WHICH THE NONCONDENSIBLES ARE LESS THAN 5% OF THE GAS CONCENTRATION. THIS LIMIT IS SUGGESTED BY EXPERIMENTS REPORTED IN COLLIER (CONVECTIVE BOILING AND CONDENSATION, FIG. 10.4 OF REF. 4), A COPY OF WHICH IS IN THE AC06 FILE. HOWEVER, THESE EXPERIMENTS, ALONG WITH THE BSL FORMULA, CAST SOME DOUBT ON THE ACCURACY OF THE CONTAIN RESULTS EVEN FOR HIGHER NONCONDENSIBLE CONCENTRATIONS. FIG. 10.4 OF COLLIER SUGGESTS THAT THE HTC FOR CONDENSATION WITH A SIGNIFICANT NONCONDENSIBLE CONCENTRATION PLATEAUS OUT AT 3% TO 10% OF THE PURE VAPOR VALUE. THIS SUGGESTS A VALUE OF .03 X 2.E4 = 600, WHEREAS ALL WE GOT IN AC01 WAS 14. NOTE THAT THE PARAMETER REGIMES ARE VERY DIFFERENT, SO THIS IS NO PROOF THAT CONTAIN IS WRONG, BUT IT IS CAUSE FOR CONCERN AND MOTIVATION TO DO MORE TESTS, E.G., THE ONES SUGGESTED IN REPORT #AC01.

   (ADDENDUM 4/13/83: THIS TEST WAS RUN ON VERSION 120, USING THE NEW CONDENSATION MODEL, WITH MUCH BETTER RESULTS. THE TOTAL HEAT TRANSFER COEFFICIENT (AT 5 S INTO THE RUN) WAS ABOUT 900. IF WE REMOVE THE EFFECT OF THE PAINT LAYER, WE GET 1636, WHICH IS IN THE RANGE OF VALUES SUGGESTED BY COLLIER (FIGURE 10.4).

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

---

1. PROBLEM: ID NO.AC06-01 2. LEVEL: PL2 3. RESOLVED? YES
4. DESCRIPTION: THE STRUCTURE CONDENSATION MODEL IS HIGHLY INACCURATE FOR LOW CONCENTRATIONS (E.G., 5%) OF NONCONDENSIBLE GAS IN THE ATMOSPHERE.
5. DATE PROBLEM RESOLVED: 4/13/83 (NEW CONDENSATION MODEL)

CONTAIN TEST SUMMARY REPORT

1. <u>IDENT NUMBER</u>: AC08 <u>USER NAME</u>: K. D. BERGERON

2. <u>TEST LEVEL</u>: TL2

3. <u>TITLE OF TEST</u>: CONDENSATION ON STRUCTURES: EFFECT OF ORIENTATION

4. <u>CODE VERSION (DATE)</u>: 312 (3/16/82)

5. <u>ACTIVE MODULES OR OPTIONS</u>: SEE AC01

6. <u>CONTAINMENT CONFIGURATION AND SOURCES</u>: SAME AS AC01, EXCEPT THAT SINK1 WAS REPEATED THREE TIMES, ONCE AS A WALL, ONCE AS A ROOF, AND ONCE AS A FLOOR.

7. <u>TEST</u>: THE HEAT TRANSFER COEFFICIENT SHOULD BE DIFFERENT FOR THE DIFFERENT ORIENTATIONS, BECAUSE OF THE DIFFERENT CORRELATIONS USED FOR THE TREATMENT OF THE BOUNDARY LAYER.

8. <u>RESULTS OF TEST</u>: FLOORS AND ROOFS ARE TREATED EXACTLY THE SAME. THE HTC IS INCREASED TO 89.4 COMPARED WITH THE VALUE OF 14.4 FOR WALLS.

9. <u>COMMENTS</u>: FLOORS AND ROOFS SHOULD NOT BE TREATED THE SAME; THE ROOF HTC SHOULD BE CONSIDERABLY LARGER BECAUSE OF THE UNSTABLE THERMAL CONDITIONS ("COOLED PLATE FACING DOWN") WHICH LEADS TO A TURBULENT BOUNDARY LAYER. I ALSO THINK THAT A 10-METER-HIGH WALL SHOULD HAVE A LARGER (NOT SMALLER) HTC THAN THE ROOF BECAUSE OF THE HIGH REYNOLDS NUMBER ASSOCIATED WITH A LARGE, HEATED WALL; BUT I HAVE NOT YET CHECKED THIS OUT.

10. <u>SUGGESTIONS FOR ADDITIONAL TESTS</u>: TEST DEPENDENCE ON HEIT1 PARAMETER. THIS IS THE HEIGHT USED FOR THE HEAT-TRANSFER CORRELATION.

---

1. PROBLEM: ID NO.AC08-01 2. LEVEL: PL2 OR PL3 3. RESOLVED? YES
4. DESCRIPTION: ROOFS AND FLOORS ARE TREATED THE SAME IN THE CONDENSATION ROUTINE; THEY SHOULD BE TREATED WITH DIFFERENT CORRELATIONS, AND THEY SHOULD GIVE DIFFERENT HEAT TRANSFER COEFFICIENTS.
5. DATE PROBLEM RESOLVED: 9/30/82--NEW CONDENSATION MODEL; SEE AC22

==

1. PROBLEM: ID NO.AC08-02 2. PL2 OR PL3 3. RESOLVED? YES
4. DESCRIPTION: THE HTC FOR WALLS IS ONE SIXTH THAT FOR A ROOF. THIS SEEMS COUNTER-INTUITIVE, THOUGH THE REQUIRED CALCULATIONS TO CHECK THIS INTUITION HAVE NOT YET BEEN DONE.
5. DATE PROBLEM RESOLVED: 9/30/82--NEW CONDENSATION MODEL; SEE AC22

==

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: AC22(ST) USER NAME: K. D. BERGERON

2. TEST LEVEL: TL4A

3. TITLE OF TEST: FORCED AND NATURAL CONDENSATION ON STRUCTURES

4. CODE VERSION (DATE): A20 (12/10/82); 120 (2/8/83)

5. ACTIVE MODULES OR OPTIONS: NEW CONDENSATION MODEL, WITH FORCED AND NATURAL CONVECTION OPTIONS ACTIVATED, AND WITH SIMPLE CONDENSATE FILM RESISTANCE MODEL

6. CONTAINMENT CONFIGURATION AND SOURCES: SAME AS AC01, BUT AFTER 40 S FORCED CONVECTION IS APPLIED TO TWO STRUCTURES (ROOF OF CELL AND A WALL STRUCTURE) FOR WHICH CONVECTION VELOCITIES ARE INPUT

7. TEST: COMPARE HEAT TRANSFER COEFFICIENTS WITH TYPICAL UCHIDA VALUES; CHECK FILM BUILDUP LOGIC; CHECK TO SEE WHETHER THE TYPES OF PROBLEM IDENTIFIED IN THE PROBLEM REPORTS AC08-01 AND AC08-02 HAVE BEEN RESOLVED.

8. RESULTS OF TEST: THE DEBUG OPTION IN THE NEW CONDENSATION MODEL CALCULATES THE HEAT TRANSFER COEFFICIENT DIRECTLY, SO THE HAND CALCULATION DESCRIBED IN TEST REPORT AC01 IS NOT NECESSARY. IN THE NATURAL CONVECTION PERIOD, THE HEAT TRANSFER COEFFICIENTS ARE HIGHER THAN WITH THE OLD MODEL. AT T = 10 S, FOR EXAMPLE, IT IS 167 FOR STRUCTURE 5 (WALL). TO COMPARE THIS WITH THE UCHIDA CORRELATION, WE MUST SUBTRACT THE EFFECT OF THE PAINT LAYER (ANOTHER NEW FEATURE OF THE MODEL), WHICH GIVES A VALUE OF HTC = 182. THE UCHIDA VALUE IS 288, SO OUR MODEL PREDICTS A VALUE OF 63% OF THE UCHIDA CORRELATION, INDICATING THAT IT IS APPROXIMATELY THE RIGHT MAGNITUDE. THE FLOOR VALUE IS 26, WHICH IS ABOUT 1/6 OF THE WALL AND ROOF VALUES, THUS RECONCILING THE PROBLEMS IDENTIFIED IN AC08-01 AND AC08-02. THE FORCED-CONVECTION OPTION SEEMS TO WORK AS EXPECTED. THE HEAT-TRANSFER COEFFICIENTS FOR THE TWO STRUCTURES THAT HAVE CONVECTIVE VELOCITY INPUTS INCREASE FROM 114 TO 175 FOR THE RATHER MODEST VELOCITY OF 3 M/S AND INCREASE FROM 152 TO 655 FOR A VELOCITY OF 10.5 M/S. THE CONDENSATE FILM MASS IS ALSO REASONABLE.

9. COMMENTS: THE NEW CONDENSATION MODEL APPEARS TO WORK WELL, AND ALL OF THE QUANTITATIVE PROBLEMS OF THE OLD MODEL HAVE BEEN RESOLVED BY IT (AC01-01, AC08-01, AC08-02). IT SHOULD ALSO BE NOTED THAT IN MARCH 1982, PRELIMINARY DATA FROM THE BLIND CODE-VALIDATION EXERCISE, INVOLVING A REACTOR BLOWDOWN EXPERIMENT AT THE HDR FACILITY IN GERMANY, INDICATED THAT THE CONDENSATION MODEL PREDICTS LONG-TERM PRESSURE AND TEMPERATURE BEHAVIOR EXTREMELY WELL.

10. SUGGESTIONS FOR ADDITIONAL TESTS: SODIUM-COOLANT TESTS. TESTS INVOLVING EVAPORATION AND/OR COMPETITION BETWEEN STRUCTURES AND AEROSOLS FOR CONDENSATE.

Supporting Analysis: AC Series - Condensation Heat Transfer to Structures

The Uchida correlation referenced in the test reports for the AC series is based on a limited number of experiments in small geometries, under conditions of natural convection.[2] Nonetheless, it has been widely used in reactor-safety codes, and appears to be reasonably accurate for modeling post-blowdown stages of condensation heat transfer. It is relevant, therefore, to use it for determining whether condensation models are in the right "ball park". In fact, the discrepancy between CONTAIN and the Uchida correlation was the key observation which led to the revision of the model (see AC01.) The Uchida correlation is presented in Reference 5 as

$$h_c = 450 \, (M_s/M_a)^{.8} \tag{3.1-6}$$

where M_s is the steam mass (vapor only), and M_a is the mass of air. For example, for the case discussed in AC22(ST), the mass of H_2O in the atmosphere at $t = 10$ s is 1.45E5 kg, with a quality of .27, for a total steam mass of 3.91E4 kg. The noncondensible mass is 6.85E4 kg, which results in $h_c = 288$. The value calculated for a typical wall structure is 167, but that includes the paint layer resistance, which does not apply to the Uchida experiments. The paint heat transfer coefficient assumed is 2000, so that the proper value to compare with Uchida is 182:

$$\frac{1}{167} - \frac{1}{2000} = \frac{1}{182}$$

References:

1. Tagami, T., unpublished data, 1965.

2. Uchida, H. et al, Proceedings of the International Conference on the Peaceful Uses of Atomic Energy (A/CONF.28/P436).

3. Bird, R. B., W. E. Steward, and E. N. Lightfoot, Transport Phenomena (New York: John Wiley & Sons, 1960).

4. Collier, J. G., Convective Boiling and Heat Transfer (New York: McGraw-Hill, 1972).

5. Slaughterbeck, D. C., "Review of Heat Transfer Coefficients for Condensing Steam in a Containment Building Following a Loss of Coolant Accident," IN-1388 (Idaho Nuclear Corporation, 1970).

SERIES AC STANDARD TEST INPUT DATA SET

```
&& ------------------ TEST AC22(ST) -------------------------------

&& TEST INPUT FOR NEW CONDENSATION MODEL--FORCED CONVECTION AND DEBUG

CONTROL=9 1 2 2 2 1 0 0 0 0
MATERIAL
COMPOUND N2 O2 H2OL H2OV CONC FE
FISSION DUM1 DUM2
TIMES 59. 0. .2 5. 40.
            1. 5. 80. 1.

FISSION
0 2
DUM1 DUM2
1.0E8 1.0E10
2*2.5E4 EOI
TITLE
TEST ID AC22(ST); NEW CONDENSATION MODEL
FORCED CONVECTION IN SECOND TIME ZONE ONLY (AFTER 40 SEC)
THERMAL
FLOWS
DEBUG=1 ATMCON 0. 60.
PRHEAT
PRFLOW


CELL=1
CONTROL=20 0 0 7 6
  0 0 1 14 0
  0 0 0 0 0 0
  0 0 0 0 0 && A20 VERSION INPUT

GEOMETRY 5.95E4, 48.03


STRUC


  R1,ROOF,SPHERE,6,0,300.
  19.85,0.,300.
  19.85,19.855,19.87,19.88,20.13,20.39,20.64
  FE,FE,FE,CONC,CONC,CONC

  F1,FLOOR,SLAB,4,0,300.
  19.85,0.,300.,1.24E3
  0.,.005,1.33,2.67,4.
  CONC,CONC,CONC,CONC

  W1,WALL,CYLINDER,6,0,300.
  38.1,0.,300.,38.1
  19.85,19.855,19.87,19.88,20.24,20.6,20.95
  FE,FE,FE,CONC,CONC,CONC
```

```
 W2,WALL,CYLINDER,6,0,300.
  38.1,0.,300.,38.1
  19.85,19.855,19.87,19.88,20.24,20.6,20.95
  FE,FE,FE,CONC,CONC,CONC

 SINK1,WALL,SLAB,3,1,300.
  10.,0.,1.41E4
  0.,.005,.300,.305
  CONC,CONC,CONC

 SINK2,WALL,SLAB,3,1,300.
  10.,0.,1.4E3
  0.,.001,.00535,6.35E-2
  FE,FE,FE

 SINK3,WALL,SLAB,3,1,300.
  10.,0.,1.61E4   && AREA REDUCED COMPARED TO AC01, ETC. AGREES WITH CONTEMPT
  0.,.001,.003,3.81E-3
  FE,FE,FE


ATMOS=3
1.003E5 294.2
N2=.795 O2=.195 H2OV=1.E-5 && ESSENTIALLY DRY INITIAL ATMOSPHERE
  CONDENSE                     &&   SURFACE CONDENSATION ACTIVATED
  FORCED 2 2      && FORCED CONVECTION IN SECOND TIME ZONE
  1 3.0
  5 10.5


SOURCE=1
  H2OV=14
  IFLAG=2
   T=  0.      0.2     0.7     1.2     2.2     3.2     4.2     8.2     10.2
 15.2   20.2   22.7   23.2   1000.

MASS= 0.691E4 2.971E4 2.717E4 2.457E4 1.964E4 1.693E4 1.516E4
      0.965E4 0.827E4 0.381E4 0.216E4 0.011E4 0. 0.

ENTH= 1.131E6 1.126E6 1.127E6 1.131E6 1.117E6 1.113E6 1.108E6
      1.142E6 1.138E6 1.102E6 0.629E6 0.454E6 0. 0.
EOI
EOF
```

3.1.3 Series HS - Transient Heat Conduction in Structures

This test series tested the routines in CONTAIN dealing with transient heat conduction within solids. The results from CONTAIN were checked using single purpose computer codes designed specifically to deal with conductive heat transfer. These tests evaluated the heat transfer within the different structural shapes used in CONTAIN - spheres, cylinders, and slabs. In addition, time-step sensitivity and the sensitivity to different zoning configurations were investigated.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: HS01(ST), HS02 USER NAME: K. D. BERGERON

2. TEST LEVEL: TL4C

3. TITLE OF TEST: STRUCTURE HEAT TRANSFER

4. CODE VERSION (DATE): 208 (3/01/82); 312 (5/82)

5. ACTIVE MODULES OR OPTIONS: HEAT TRANSFER ONLY. FLOWS IS OFF.

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH THREE STRUCTURAL ELEMENTS: A SLAB, A CYLINDER, AND A SPHERE. EACH CONSISTS OF TWO LAYERS OF DIFFERENT MATERIAL (URANIUM AND CONCRETE) WITH A TOTAL THICKNESS OF APPROXIMATELY 1.2M. INITIALLY, THE STRUCTURES ARE AT A UNIFORM TEMPERATURE (300 K), AND THEN (AT TIME = 0) THEY ARE HEATED BY A UNIFORM CONVECTIVE ATMOSPHERE AT 500 K, EITHER ON THE INSIDE (HS02) OR THE OUTSIDE (HS01) OF THE STRUCTURE. THE UNHEATED SIDE IS EITHER ADIABATIC (HS02) OR CONVECTIVE AT 300 K (HS01). TEMPERATURES INSIDE THE STRUCTURES ARE FOLLOWED FOR TIMES UP TO 1.E7 S.

7. TEST: COMPARE PREDICTIONS OF CONTAIN WITH THOSE OF SINDA, A WELL ESTABLISHED FINITE-ELEMENT HEAT-TRANSFER CODE. (ADDENDUM: 6/22/82. TO RESOLVE THE DISCREPANCY, A THIRD CODE WAS USED FOR THE SAME PROBLEM. THIS WAS CONDUCT, WRITTEN BY B. BULMER OF SANDIA AND EXTENSIVELY USED FOR THE PAST TEN YEARS AT SANDIA. IT IS A ONE-DIMENSIONAL HEAT-CONDUCTION CODE, WHICH WAS RUN ON NOS.)

8. RESULTS OF TEST: THE CONTAIN RESULTS WERE SIGNIFICANTLY DIFFERENT FROM THE SINDA RESULTS. THE TEMPERATURE PROFILES HAD APPROXIMATELY THE RIGHT SHAPE AND THE RIGHT ASYMPTOTIC TEMPERATURES, BUT THE HEAT WAVE MOVED FASTER IN CONTAIN THAN IN SINDA. THE DIFFERENCE WAS FOUND TO BE EQUIVALENT TO AN ERROR IN THERMAL DIFFUSIVITY OF APPROXIMATELY 40% (INCREASE.) CALCULATIONS OF EFFECTIVE STRUCTURE/ATMOSPHERE HEAT-TRANSFER COEFFICIENT SHOWED THAT CONTAIN WAS DOING THAT PORTION OF THE HEAT TRANSFER RIGHT: THE VALUE 2.25, WHICH WAS THE CODE DEFAULT VALUE, WAS OBTAINED. CALCULATIONS OF EFFECTIVE DIFFUSIVITY WITHIN THE STRUCTURE (FOR THE SLAB CASE) RESULTED IN VALUES THAT WERE APPROXIMATELY WHAT THEY SHOULD HAVE BEEN AND CERTAINLY NOT 40% TOO HIGH.

(ADDENDUM: 6/22/82. THE CONDUCT RUNS RESOLVED THE PROBLEM. CONDUCT AGREED QUITE PRECISELY WITH CONTAIN AND DISAGREED WITH SINDA. IT WAS DETERMINED THAT THE SINDA RUNS WERE IN ERROR BECAUSE OF A POOR ZONING SCHEME. ONE MINOR DISCREPANCY BETWEEN CONTAIN AND CONDUCT WAS IDENTIFIED, HOWEVER, FOR HEMISPHERICAL STRUCTURES. THIS WAS TRACED TO A FACTOR-OF-TWO ERROR IN THE VOLUME FORMULA FOR HEMISPHERES. AFTER IT WAS CORRECTED, CONTAIN AGREED PRECISELY WITH CONDUCT FOR ALL CASES AND ALL TIMES.)

9. COMMENTS: THESE TESTS ARE A RELATIVELY RIGOROUS VALIDATION OF STRUCTURE HEAT TRANSFER IN CONTAIN.

10. SUGGESTIONS FOR ADDITIONAL TESTS: THE RADIATIVE HEAT TRANSFER OPTION HAS NOT BEEN TESTED, NOR HAS HEAT TRANSFER FROM THE POOL TO THE STRUCTURES.

1. PROBLEM: ID NO.HS01-01 2. LEVEL: PL2 3. RESOLVED? YES
4. DESCRIPTION: CONTAIN SEEMS TO PROPAGATE HEAT IN STRUCTURES AT A SIGNIFICANTLY HIGHER RATE (EQUIVALENT TO AN INCREASE OF 40% IN THE DIFFUSIVITY) THAN SINDA, A WELL VALIDATED FINITE-ELEMENT CODE.
5. DATE PROBLEM RESOLVED: 5/82; SINDA CALCULATIONS WERE INCORRECT.

1. PROBLEM: ID NO.HS01-02 2. LEVEL: PL1 3. RESOLVED? YES
4. DESCRIPTION: WITH MULTIPLE TIME ZONES, IT CAN BE DIFFICULT TO GET OUTPUT AT TIMES DESIRED. THE FIRST EDIT IN ALL TIME ZONES EXCEPT THE FIRST OCCURS AT TSTOP + TIMINC, WHERE TSTOP IS THE LAST TIME ZONE VALUE. FURTHERMORE, THERE IS NO EDIT AT TSTOP, UNLESS IT IS AN INTEGRAL NUMBER OF TIMINC FROM THE FIRST EDIT IN THAT ZONE. A SIMPLER SCHEME, IN WHICH THERE IS ALWAYS AN EDIT AT TSTOP, IS HIGHLY DESIRABLE.
5. DATE PROBLEM RESOLVED: 4/2/82

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: HS03 USER NAME: K. D. BERGERON

2. TEST LEVEL: TL2, TL4C

3. TITLE OF TEST: STRUCTURE HEAT TRANSFER: TIME-STEP SENSITIVITY

4. CODE VERSION (DATE): 312 (3/11/82)

5. ACTIVE MODULES OR OPTIONS: SAME AS HS01

6. CONTAINMENT CONFIGURATION AND SOURCES: SAME AS HS01

7. TEST: CHANGE THE TIME STEP TO ONE TENTH OF HS01 AND LOOK FOR DIFFERENCES.

8. RESULTS OF TEST: OUTPUT AT TIME = 1.1E6 S WAS ANALYZED. THIS WAS IN THE PERIOD SHOWING THE LARGEST DISCREPANCIES FROM SINDA RESULTS. THERE WERE VIRTUALLY NO DIFFERENCES IN PREDICTED TEMPERATURE BETWEEN HS01 AND HS03. (TYPICAL DIFFERENCES WERE LESS THAN .5 K.)

9. COMMENTS: THE DISCREPANCY FROM SINDA IS NOT DUE TO TOO LONG A TIME STEP.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: HS04 USER NAME: K. D. BERGERON

2. TEST LEVEL: TL3

3. TITLE OF TEST: STRUCTURE HEAT TRANSFER: ZONING SENSITIVITY

4. CODE VERSION (DATE): 312 (4/1/82)

5. ACTIVE MODULES OR OPTIONS: SAME AS HS01

6. CONTAINMENT CONFIGURATION AND SOURCES: THE STRUCTURES ARE ZONED MORE FINELY THAN IN TEST HS01. A TOTAL OF 39 NODES (COMPARED WITH 23) WERE USED.

7. TEST: LOOK FOR DIFFERENCES FROM HS01 RESULTS DUE TO ZONING SENSITIVITY. TEMPERATURES AT R = .101, .195, AND 1.19 WERE INSPECTED FOR TIMES UP TO 1.E7 S.

8. RESULTS OF TEST: ONLY SMALL DIFFERENCES WERE FOUND. THE LARGEST TEMPERATURE DIFFERENCES OBSERVED WERE 3 TO 4 K AT R = .101 AND R = .195 FOR SPHERES AND CYLINDERS. OTHER POSITIONS AND GEOMETRIES SHOWED MUCH SMALLER DIFFERENCES.

9. COMMENTS: THERE ARE VIRTUALLY NO ZONING SENSITIVITIES ON THE SCALE OF THE DISCREPANCIES BETWEEN THE SINDA AND CONTAIN RESULTS FOUND IN TEST HS01 AND HS02.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

Supporting Analysis: HS Series - Transient Heat Conduction in Structures

The CONTAIN-CONDUCT comparisons are the key results of these tests. These are shown in Figures HS-01 through HS-06. Among these are two cases where discrepancies are seen. Figure HS-04 shows that the SINDA calculation was not in agreement with CONTAIN. As discussed in the Test Summary Report, the error was in the SINDA analysis, which used a poor zoning scheme. Figure HS-05 shows the results before the coding error for sphere volume was corrected. Figure HS-06 shows the results after the error was corrected.

In May 1982, the heat transfer coefficient, HAS, hardwired into the code for this type of problem (CONDENSE not on) was changed from 2.25 to 6.08. Therefore, it will not be possible to generate calculations to be compared with Figures HS-01 through HS-06 unless the value of HAS is changed with updates.

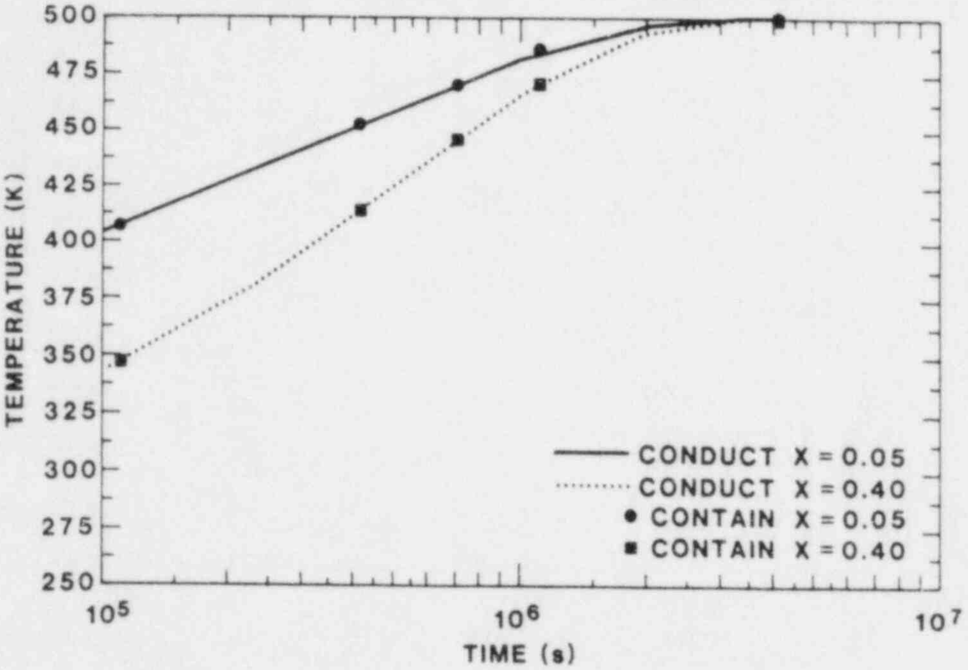

Figure HS-01 Heat conduction for slabs with adiabatic outer boundary (Test HS02).

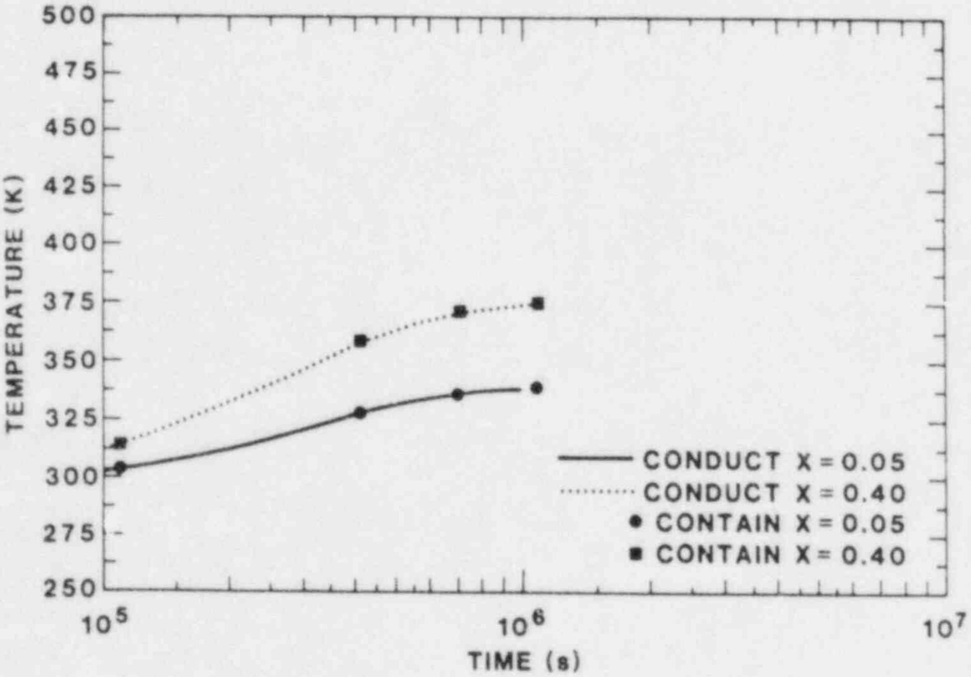

Figure HS-02 Heat conduction for slabs with convective outer boundary (Test HS01).

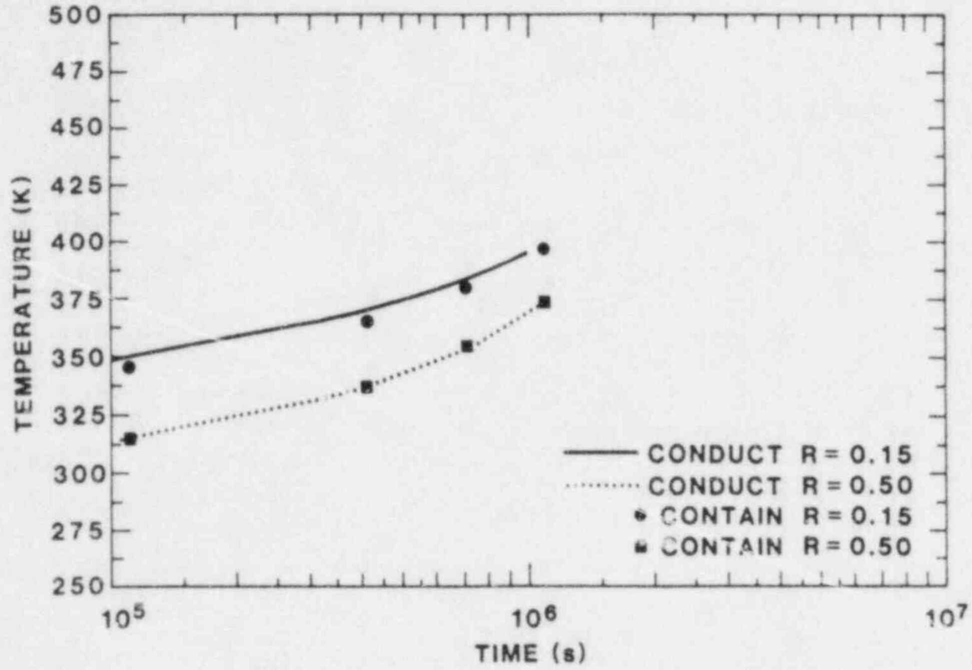

Figure HS-03 Heat conduction for cylinders with adiabatic outer boundary (Test HS02).

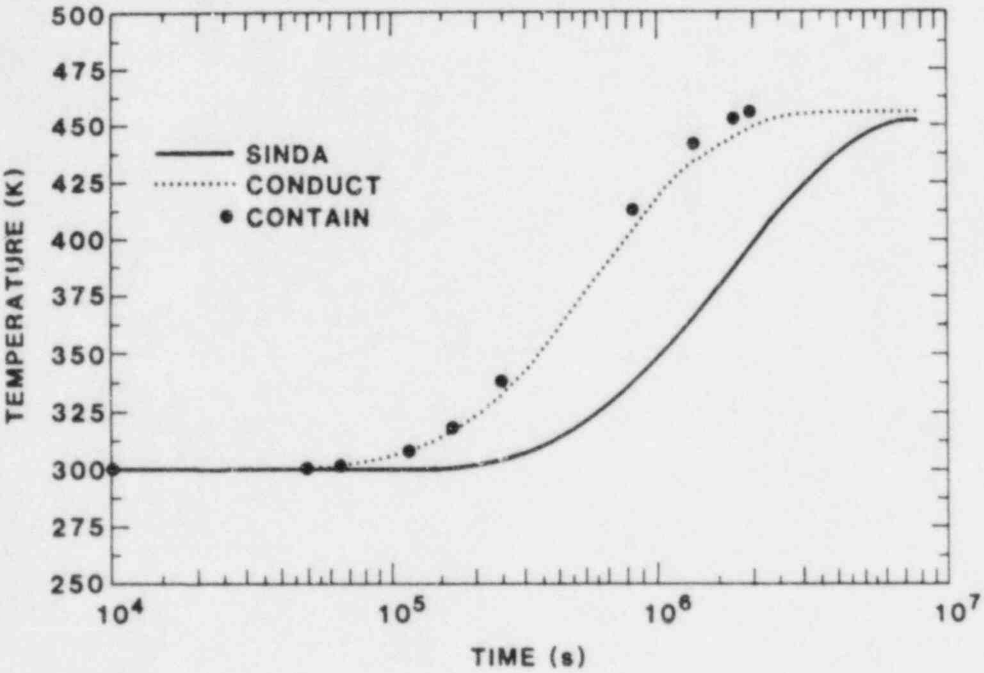

Figure HS-04 Comparison of CONTAIN, CONDUCT, and SINDA results at R = 0.101 for cylinders with convective outer boundary (Test HS01).

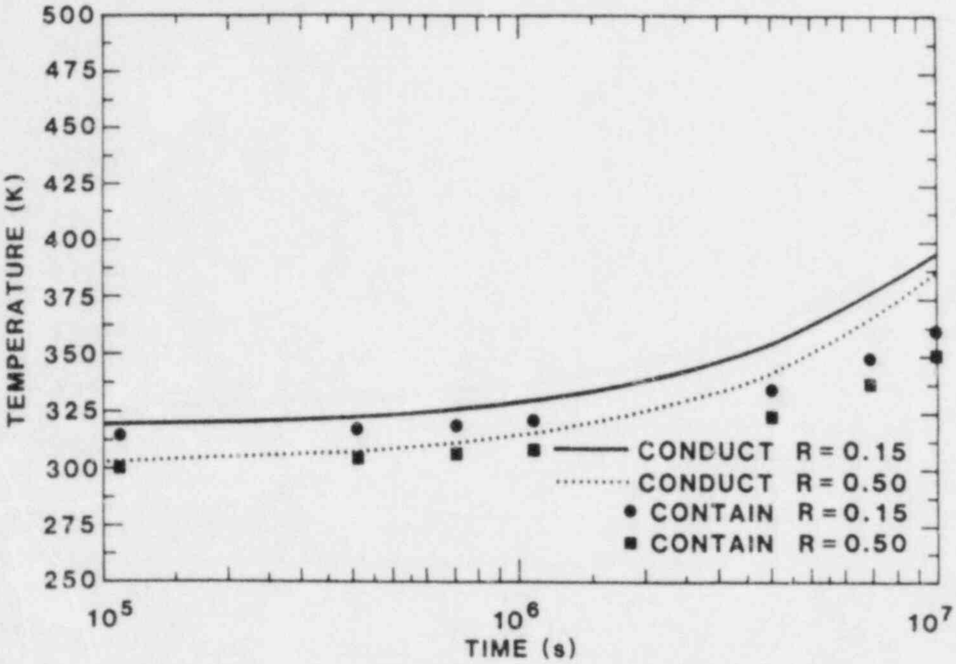

Figure HS-05 Comparison of CONTAIN and CONDUCT results for spheres with adiabatic outer boundary before correction of CONTAIN coding error (Test HS02).

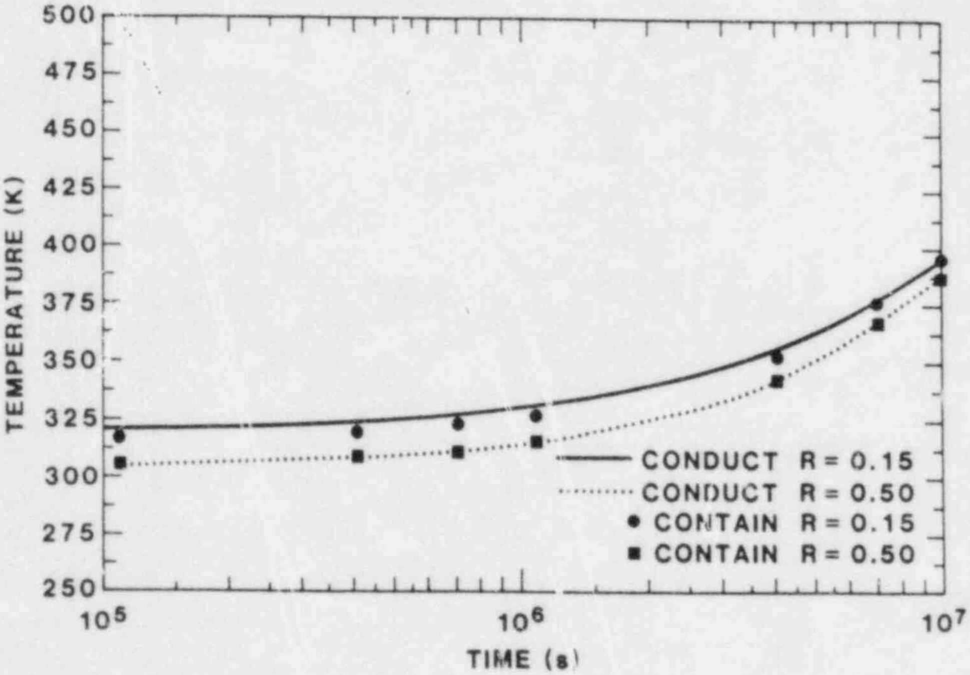

Figure HS-06 Comparison of CONTAIN and CONDUCT results for spheres with adiabatic outer boundary after correction of CONTAIN coding error (Test HS02).

SERIES HS STANDARD TEST INPUT DATA SET

```
   CONTAIN TEST HS01(ST) --- STRUCTURE HEAT TRANSFER ---
CONTROL=9 1 2 4 2 1 0 0 0 0
MATERIAL
COMPOUND U,CONC,O2
FISSION DM1 DM2
TIMES 100. 0.
&& -------------------TIME ZONES------------
  1.E2  2.E3  1.E4
  1.E3  3.E4  1.E5
  1.E4  3.E5  1.E6
  1.E5  3.E6  1.E7
&&  --------------------------------
  1.
PRHEAT
FISSION
  0 2
  DM1 DM2
  1.E8 1.E9
2*2.5E4
  EOI
TITLE
CONTAIN TEST-----IDENT HS01(ST)
STRUCTURE HEAT TRANSFER 2/26/82 ----CONVECTIVE OUTER BOUNDARY---
THERMAL
CELL=1
CONTROL=18
0 0 3 23
0 0 0 0 0 0
0 0 0 0 0
0 0 0
GEOMETRY 1. 1.
ATMOS=1  1.E5

300.  && ------------------CELL TEMPERATURE
O2=1.0
STRUC
SLAB,WALL,SLAB,23,8
300.  && ----------------------STRUCTURE INITIAL TEMPERATURE
0. 0.
500.  && ----------------------OUTER WALL TEMPERATURE (CONVECTIVE)
1.
&& ---WALL ZONES-----
 .1 .1005 .1015  && ------------------NODE 2 AT R=.101
 .105 .12 .14 .16 .18 .19 .20   && ---------NODE 9 AT R=.195
 .21 .24 .3 .36 .44 .56  && ----------NODE 15 AT R=.5
 .7 .85 .9 1.0 1.08 1.15 1.18 1.2  && ------NODE 23 AT R=1.19
U U U U U U U U
CONC CONC CONC CONC CONC
CONC CONC CONC CONC CONC
CONC CONC CONC CONC
```

```
CYLINDER,WALL,CYLINDER,23,8
300.  && ----------------------STRUCTURE INITIAL TEMPERATURE
0. 0.
500.  && ----------------------OUTER WALL TEMPERATURE (CONVECTIVE)
1.
&& ---WALL ZONES-----
 .1 .1005 .1015   && ------------------NODE 2 AT R=.101
 .105 .12 .14 .16 .18 .19 .20  && ---------NODE 9 AT R=.195
 .21 .24 .3 .36 .44 .56  && ----------NODE 15 AT R=.5
 .7 .85 .9 1.0 1.08 1.15 1.18 1.2  && ------NODE 23 AT R=1.19
U U U U U U U U U
CONC CONC CONC CONC CONC
CONC CONC CONC CONC CONC
CONC CONC CONC CONC

SPHERE,WALL,SPHERE,23,8
300.  && ----------------------STRUCTURE INITIAL TEMPERATURE
0. 0.
500.  && ----------------------OUTER WALL TEMPERATURE (CONVECTIVE)
&& ---WALL ZONES-----
 .1 .1005 .1015  && ------------------NODE 2 AT R=.101
 .105 .12 .14 .16 .18 .19 .20  && ---------NODE 9 AT R=.195
 .21 .24 .3 .36 .44 .56  && ----------NODE 15 AT R=.5
 .7 .85 .9 1.0 1.08 1.15 1.18 1.2    ------NODE 23 AT R=1.19
U U U U U U U U U
CONC CONC CONC CONC CONC
CONC CONC CONC CONC CONC
CONC CONC CONC CONC

EOF
```

3.1.4 Series VA - Sodium- and Water-Vapor Thermodynamics

This test series tested CONTAIN's predictions of the behavior of atmospheres containing mixtures of noncondensible gases and either sodium vapor or water vapor. Tests VA01, -02, -03, -07, and -08 used mixtures of sodium vapor and nitrogen. Tests VA04, -05, and -06 used water vapor with nitrogen. These tests are somewhat similar to the AA Series tests, but they extend the area examined into the near-superheat and superheat regimes.

The initial tests in this series showed that CONTAIN's predictions of near-superheat or superheat conditions involving sodium vapor were substantially in error. Checks of the coding revealed several problems. These problems were caused by an incorrect units conversion factor and by the way certain sodium thermodynamic properties were determined. Coding updates corrected the problems. The corrected coding gave fairly good results.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: VA01, VA02(ST), VA03, VA07, VA08(ST) USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: SODIUM-VAPOR THERMODYNAMICS
4. CODE VERSION (DATE): 324 (6-1 THRU 7-7-82)
5. ACTIVE MODULES OR OPTIONS: ATMOSPHERE THERMODYNAMICS
6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE ADIABATIC CELL WITH A VOLUME OF 2477.66 CUBIC METERS. THE CELL IS INITIALLY FILLED WITH NITROGEN GAS AT 1.0E5 PA PRESSURE. THE INITIAL GAS TEMPERATURE RANGES FROM 298.0 K TO 1100.0 K, DEPENDING ON THE TEST. VARYING QUANTITIES OF SODIUM VAPOR AT 1154.0 K (SATURATED) ARE INJECTED INTO THE CELL. TEST CONDITIONS WERE VARIED SO AS TO HAVE END STATES IN BOTH THE SATURATED AND SUPERHEATED REGIONS.
7. TEST: COMPARE THE FINAL TEMPERATURE AND PRESSURE IN THE CELL AS PREDICTED BY CONTAIN WITH PREDICTIONS FROM SEPARATE HAND ANALYSES OF THESE CONDITIONS.
8. RESULTS OF TEST: TESTS VA01 AND VA08 RESULTED IN AN END STATE WITH SATURATION CONDITIONS. THE KEY PARAMETERS FOR THESE TESTS WERE AS FOLLOWS:

	NITROGEN		SODIUM VAPOR	
TEST	TEMP, K	KG-MOLES	TEMP, K	KG-MOLES
VA01	298.0	100.0	1154.0	6.0
VA08	890.0	33.48	1154.0	6.0

THE CONDITIONS FOR VA01 GAVE AN END STATE WHERE MOST OF THE INJECTED SODIUM CONDENSED, LEAVING ONLY A SMALL QUANTITY OF SODIUM VAPOR IN THE ATMOSPHERE. CASE VA08 HAD AN END STATE WHEREIN THE SODIUM VAPOR QUALITY WAS ON THE ORDER OF 98%. THE FOLLOWING TABLE GIVES THE CONTAIN RESULTS AND THOSE OF THE HAND CALCULATIONS:

	CONTAIN RESULTS					
TEST	W/O UPDATE		W/ UPDATE		HAND CALCULATIONS	
	TEMP, K	PRESS, PA	TEMP, K	PRESS, PA	TEMP, K	PRESS, PA
VA01	604.5	2.028E5	591.8	1.987E5	597.1	2.004E5
VA08	1646.7	2.957E5	997.2	1.310E5	992.5	1.298E5

THESE RESULTS SHOW THAT CONTAIN PREDICTIONS FOR THE CASE OF LOW SODIUM VAPOR CONTENT MATCHED THOSE OF THE HAND CALCULATIONS QUITE WELL. THE RESULTS FOR THE NEAR-SUPERHEAT CONDITIONS WERE SUBSTANTIALLY IN ERROR PRIOR TO THE CODING UPDATE. THE UPDATE CORRECTED THE PROBLEM.

TESTS VA02, VA03, AND VA07 HAD INITIAL CONDITIONS WHICH WOULD GIVE SUPERHEATED VAPOR END STATES FOR THE SYSTEM. THE FOLLOWING TABLE GIVES THESE INITIAL CONDITIONS:

	NITROGEN		SODIUM VAPOR	
TEST	TEMP, K	KG-MOLES	TEMP, K	KG-MOLES
VA02	1100.0	27.09	1154.0	6.0
VA03	1100.0	27.09	1154.0	3.0
VA07	920.0	32.39	1154.0	6.0

THE SUPERHEAT CASES GAVE THE FOLLOWING RESULTS:

	CONTAIN RESULTS					
TEST	W/O UPDATE		W/ UPDATE		HAND CALCULATIONS	
	TEMP, K	PRESS, PA	TEMP, K	PRESS, PA	TEMP, K	PRESS, PA
VA02	2233.8	8.449E5	1185.9	1.317E5	1171.6	1.301E5
VA03	1602.2	2.362E5	1142.9	1.154E5	1139.8	1.151E5
VA07	1646.7	2.957E5	997.2	1.310E5	992.5	1.298E5

THIS TABULATION SHOWS THAT THE UNMODIFIED CODE SUBSTANTIALLY OVERPREDICTED THE END STATE TEMPERATURES AND PRESSURES FOR THESE SUPERHEATED SODIUM CASES. THE UPDATES, HOWEVER, HAVE CORRECTED THE PROBLEM, AND THE CODE RESULTS ARE NOW IN CLOSE AGREEMENT WITH THOSE OF THE HAND CALCULATIONS.

9. COMMENTS: THE CODING IN VERSION 324 GIVES REASONABLE PREDICTIONS OF THE TEMPERATURE AND PRESSURE OF AN ATMOSPHERE CONTAINING SATURATED SODIUM VAPOR IF THE QUALITY (VAPOR MASS/LIQUID-PHASE MASS) IS FAIRLY LOW. ITS PREDICTIONS FOR THE HIGH VAPOR QUALITY REGIME AND FOR SUPERHEATED VAPOR END STATES ARE SIGNIFICANTLY IN ERROR.

THE UPDATES TO THE CODING HAVE CORRECTED THE PROBLEM. THE PROBLEM WAS ASSOCIATED WITH THE WAY SODIUM THERMODYNAMIC PROPERTIES WERE DETERMINED. IN ADDITION, A UNITS CONVERSION FACTOR WAS WRONG. THE CODE UPDATE HAS REVISED THE MANNER IN WHICH THE PROPERTIES DATA ARE HANDLED AND HAS ELIMINATED THE CONVERSION FACTOR PROBLEM.

STEAM THERMODYNAMICS TESTS: THE ERRONEOUS RESULTS FROM CONTAIN FOR THE SUPERHEATED SODIUM VAPOR TEST CASES PROMPTED ADDITIONAL TESTS USING STEAM INSTEAD OF SODIUM VAPOR. TEST VA04 INVESTIGATED HIGH QUALITY SATURATED CONDITIONS, WHILE VA05 AND VA06 INVESTIGATED SUPERHEATED END STATES. IN ALL THREE TESTS THE CONTAIN RESULTS CLOSELY MATCHED THOSE FROM HAND ANALYSES (NO UPDATES NEEDED). THUS, THE PROBLEMS DISCUSSED ABOVE WERE UNIQUE TO THE SODIUM VAPOR TESTS. THE WATER VAPOR TESTS INCLUDED HERE ARE SIMILAR TO THE AA0- TEST SERIES, BUT THEY EXTEND THE RANGE INTO THE SUPERHEAT REGION.

10. <u>SUGGESTIONS FOR ADDITIONAL TESTS</u>: EXAMINE A SITUATION WHEREIN THE END-STATE QUALITY IS IN THE RANGE OF 30 TO 80% IN ORDER TO TEST THE PRESENT CODING IN THIS RANGE.

==

1. PROBLEM: ID NO. VA01 2. LEVEL: PL3 3. RESOLVED? YES
4. DESCRIPTION: THE CODE SUBSTANTIALLY OVERPREDICTS ATMOSPHERE TEMPERATURES AND PRESSURES FOR CASES WITH HIGH QUALITY SATURATED SODIUM VAPOR OR SUPERHEATED SODIUM VAPOR. AN UPDATE TO THE CODE THAT CORRECTS THIS ERROR IS AVAILABLE.
5. DATE PROBLEM RESOLVED: 6/29/82

==

Supporting Analysis: VA Series - Sodium- and Water-Vapor Thermodynamics

In these tests the initial conditions in a nitrogen-filled cell are known. Sodium vapor or water vapor is injected into the cell at a specified temperature. The hand calculations predict the mixed-atmosphere conditions at the end of the vapor-injection period.

The system energy balance is:

Energy In - Energy Out = Change in Stored Energy

Energy In $= \eta_{na} h_{na,s}$

Energy Out = 0

Change in Stored Energy = Final Energy - Initial Energy

$$= \eta_{n_2} u_{n_2,f} + \eta_{na} u_{na,f} - \eta_{n_2} u_{n_2,i} \qquad (3.1\text{-}7)$$

where

η = number of moles

h = enthalpy

u = internal energy

and the following subscripts are used:

n_2 = nitrogen

na = sodium

f = final condition

i = initial condition of noncondensible gas

s = source condition

Combining terms

$$\eta_{na} h_{na,s} - 0 = \eta_{n_2} u_{n_2,f} + \eta_{na} u_{na,f} - \eta_{n_2} u_{n_2,i} \qquad (3.1\text{-}8)$$

A. For Saturated End-State Conditions:

Allowing for the possibility of vapor condensation and denoting the liquid and gas phases by (f) and (g), respectively

$$E_{na,f} = \eta_{na} u_{na,f} = (1 - X)\eta_{na} u_{na(f),f} + X\eta_{na} h_{na(g),f} - X\eta_{na} (pv)_{na(g),f} \quad (3.1\text{-}9)$$

Note also that u = h - pv

where

$E_{na,f}$ = final energy of the sodium

X = quality = fraction of sodium mass that is saturated vapor

ρ = partial pressure, Pa

v = specific volume of vapor or gas

The overall energy balance equation becomes

$$\eta_{na} h_{na,s} = \eta_{n_2} (h - pv)_{n_2,f} + (1 - X)\eta_{na} u_{na(f),f} + X\eta_{na} (h - pv)_{na(g),f} - \eta_{n_2} (h - pv)_{n_2,i} \quad (3.1\text{-}10)$$

Separating knowns and unknowns gives

$$\eta_{na} h_{na,s} + \eta_{n_2} (h\text{-}pv)_{n_2,i} = \eta_{n_2} (h\text{-}pv)_{n_2,f} + (1 - X)\eta_{na} u_{na(f),f} + X\eta_{na} (h - pv)_{na(g),f} \quad (3.1\text{-}11)$$

Note that

$$X = \frac{\eta_{na(g)}}{\eta_{na(total)}} \quad (3.1\text{-}12)$$

and

$$v_{na}(g) = \frac{V}{\eta_{na(g)}} \tag{3.1-13}$$

Therefore

$$X = \frac{V}{v_{na(g)}\eta_{na(total)}} \tag{3.1-14}$$

where V = total cell volume. The nitrogen can be treated as a perfect gas: $pv = RT$. For sodium vapor, pressure can be expressed as a function of temperature.

The solution is found by iterating on final temperature and by using the corresponding properties at that final temperature.

The final system pressure is

$$P_f = p_{sat(na,f)} + \frac{\eta_{n_2} RT_f}{V} \tag{3.1-15}$$

B. For Superheated End-State Conditions:

For superheat, X = 1.0 and Na vapor can be treated as a perfect gas.

The final system energy can be expressed as

$$\eta_{n_2}(h - RT)_{n_{2,f}} + \eta_{na}(h - RT)_{na,f} = \eta_{n_2} h_{n_{2,f}} + \eta_{na} h_{na(g),f} - (\eta_{n_2} + \eta_{na})RT_f \tag{3.1-16}$$

Energy balance gives

$$\eta_{na} h_{na,s} = \eta_{n_2} h_{n_{2,f}} + \eta_{na} h_{na(g),f} - (\eta_{n_2} + \eta_{na})RT_f - \eta_{n_2}(h - RT)_{n_{2,i}} \tag{3.1-17}$$

The end-state temperature is found by successive iterations. The final pressure is

$$P_f = \frac{(\eta_{n_2} + \eta_{na})RT_f}{V} \qquad (3.1\text{-}18)$$

SERIES VA STANDARD TEST INPUT DATA SETS

```
&& -------------VA02(ST) DATA FILE ------------------
CONTROL=9 1 4 1 4 2 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL NA2O
H2O H2OV H2OL
FISSION
TE132 I132
I133 XE133
TIMES 50.0 0.0 1.0 1.0 40.00 1.0
FLOWS
FISSION 0 2 2
TE132 I132
I133 XE133
1.0E5 2.0E5
1.0E5 1.0E6
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 1.0 1.0
EOI
TITLE
                SODIUM VAPOR INJECTION INTO N2  ATMOSPHERE TESTS
   CASE VA02(ST):  INJECTION OF 6.0 KG-MOLES (137.94 KG) OF SODIUM INTO
       N2 FILLED CELL.  NO HEAT STRUCTURES, ADIABATIC SYSTEM.
           N2 INITIALLY AT 1100 K.
FAST
CELL =1
CONTROL=17 0 0 0 0 0 0 1 2 0 0 0 0 0 0 0 0
GEOMETRY 2477.66 10.0
ATMOS=1
1.000E5  1100.0
N2=1.0000
&& ------ INJECTION OF NAV; 68.970 KG IN 10 SECONDS ------------------
SOURCE=1
NAV=2
IFLAG=1
T=20.0 30.0
MASS=13.794 0.0
TEMP=1154.0 1154.0
EOI
ATMCHEM
EOF
```

```
&& -------------VA08(ST) DATA FILE ------------------
CONTROL=9 1 4 1 4 2 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL NA2O
H2O H2OV H2OL
FISSION
```

```
TE132 I132
I133 XE133
TIMES 50.0 0.0 1.0 1.0 25.00 1.0
FLOWS
FISSION 0 2 2
TE132 I132
I133 XE133
1.0E5 2.0E5
1.0E5 1.0E6
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 1.0 1.0
EOI
TITLE
                 SODIUM VAPOR INJECTION INTO N2  ATMOSPHERE TESTS
   CASE VA08(ST):  INJECTION OF 6.0 KG-MOLES (137.94 KG) OF SODIUM INTO
       N2 FILLED CELL.  NO HEAT STRUCTURES, ADIABATIC SYSTEM.
           N2 INITIALLY AT 890 K.
FAST
CELL =1
CONTROL=17 0 0 0 0 0 0 1 2 0 0 0 0 0 0 0 0 0
GEOMETRY 2477.66 10.0
ATMOS=1
1.000E5  890.0
N2=1.0000
&& ------ INJECTION OF NAV; 137.94 KG IN 10 SECONDS -----------------
SOURCE=1
NAV=2
IFLAG=1
T=10.0 20.0
MASS=13.794 0.0
TEMP=1154.0 1154.0
EOI
ATMCHEM
EOF
```

3.2 ATMOSPHERE-CHEMISTRY TESTS

3.2.1 Series HB - Hydrogen Burns

This test series checked two features of hydrogen burns. First, these tests checked CONTAIN's predictions of the thermodynamics of hydrogen burns by comparing the code's output (cell temperatures and pressures) following a burn with results obtained from hand analyses. Second, these tests checked CONTAIN's adherence to the criteria established governing hydrogen burns. In addition, checks were made of the sensitivity of the results to variations in time-step size.

The results from these tests showed that CONTAIN's predictions of the atmosphere conditions following a hydrogen burn are quite accurate. CONTAIN also adheres well to the established burn criteria. The tests did show that using too large a calculational time step can lead to erroneous results. However, problems of this type can be avoided if reasonable care is exercised in choosing the problem time-step size.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: HB01 USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A, TL3
3. TITLE OF TEST: HYDROGEN BURN WITH HIGH HYDROGEN CONCENTRATIONS
4. CODE VERSION (DATE): 208 (2/19/82)
5. ACTIVE MODULES OR OPTIONS: HYDROGEN BURN
6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO HEAT STRUCTURES (ADIABATIC SYSTEM). NO SOURCES.
7. TEST: (1) CHECK WHETHER OR NOT THE CODE ALLOWS FOR A COMPLETE BURN FOR THE CASE OF HIGH HYDROGEN CONCENTRATIONS AND AMPLE OXYGEN. (2) COMPARE THE FINAL TEMPERATURE AND PRESSURE OF THE CELL ATMOSPHERE WITH RESULTS DETERMINED FROM SEPARATE ANALYSES.
8. RESULTS OF TEST: (1) HYDROGEN WAS BURNED COMPLETELY, AS SHOULD HAVE BEEN THE CASE FOR THESE CONDITIONS. (2) THE FINAL SYSTEM TEMPERATURE PREDICTED BY CONTAIN WAS CHECKED USING TWO DIFFERENT METHODS. THE FIRST METHOD USED TABULATED VALUES OF REACTION-PRODUCT ENTHALPIES VS TEMPERATURE TO ARRIVE AT THE FINAL SYSTEM CONDITIONS. THE INTERNAL ENERGIES OF THE REACTION PRODUCTS WERE DERIVED FROM THE ENTHALPY VALUES. AN ITERATIVE PROCESS WAS USED TO ARRIVE AT THE FINAL TEMPERATURE. THIS PROCESS PREDICTED A FINAL TEMPERATURE OF 1535.2 K FOR THE PROBLEM CONDITIONS; THE CORRESPONDING CONTAIN VALUE WAS 1526.6 K (AGREEMENT WITHIN 0.5%). THE SECOND CALCULATIONAL APPROACH USED TEMPERATURE-DEPENDENT ISOCHORIC HEAT CAPACITIES (CV) TO ARRIVE AT THE SYSTEM FINAL CONDITIONS. THIS APPROACH GAVE A FINAL TEMPERATURE OF 1526.0 K, WHICH IS ALMOST IDENTICAL TO THE CONTAIN RESULT.

FIGURE HB-01 SHOWS THE VARIOUS BURN CRITERIA WHICH ARE MODELED IN CONTAIN AND WHICH WERE USED THROUGHOUT THE HB SERIES TESTS.

9. COMMENTS: THE HAND CALCULATIONS OF FINAL SYSTEM CONDITIONS ARE IN VERY GOOD AGREEMENT WITH THE CONTAIN RESULTS. THEREFORE, CONTAIN APPEARS TO BE HANDLING THIS TYPE OF HYDROGEN BURN CORRECTLY.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

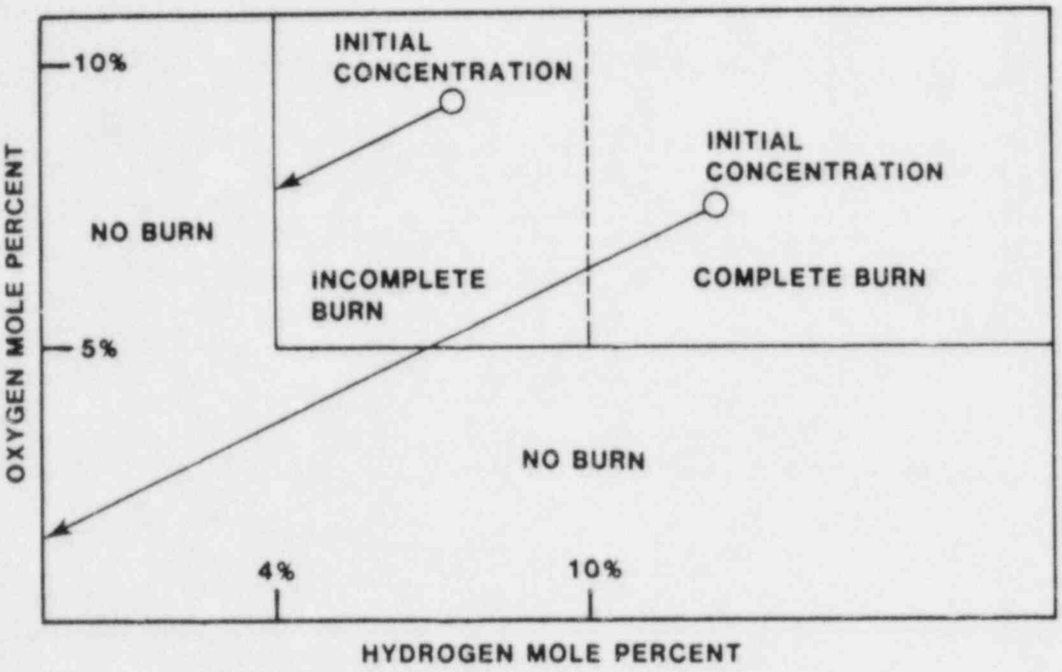

Figure HB-01 Criteria for hydrogen burn.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: HB02, HB03(ST), HB04 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A, TL3

3. TITLE OF TEST: TEST OF PARTIAL HYDROGEN-BURN CONDITIONS

4. CODE VERSION (DATE): 208 (2/25-26/82)

5. ACTIVE MODULES OR OPTIONS: HYDROGEN BURN

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO HEAT STRUCTURES. CELL INITIALLY AIR FILLED AT AMBIENT TEMPERATURE AND PRESSURE (298 K, 1.013E5 PA). HYDROGEN INJECTED AT A STEADY RATE OF 0.15 KG/S FOR 100 S.

7. TEST: (1) TEST TO SEE WHEN H2-O2 REACTION IS INITIATED.
(2) COMPARE CONTAIN AND HAND-CALCULATED RESULTS FOR FINAL SYSTEM TEMPERATURES, PRESSURES, AND ATMOSPHERE CHEMICAL COMPOSITION.
(3) CHECK EFFECT OF PROBLEM TIME-STEP SIZE.

8. RESULTS OF TEST: (1) HAND CALCULATIONS WERE MADE OF THE END STATE CONDITIONS. THIS INCLUDED PREDICTIONS OF FINAL CHEMICAL COMPOSITION, TEMPERATURE, AND PRESSURE OF THE SYSTEM. THE METHOD EMPLOYED USED TEMPERATURE-DEPENDENT HEAT CAPACITIES (CV) FOR THE CONSTITUENTS TO ESTIMATE THE END-STATE TEMPERATURE AND PRESSURE. THESE CALCULATED RESULTS WERE COMPARED TO CASE HB03 AS FOLLOWS:

	H2 REMAINING (KG)	H2 (MOLE %)	TEMP (K)	PRESS 1.0E5 PA)
CALC.--	4.07	4.0	1364.5	5.1174
CONTAIN	4.07	4.0	1371.2	5.1427

THE VALUES FROM THE TWO METHODS COMPARE QUITE WELL. THE H2-O2 REACTION STARTED WHEN THE H2 CONCENTRATION REACHED 4 MOLE %. THE H2 IN EXCESS OF 4% WAS BURNED PER THE BURN CRITERIA. THE TEMPERATURE AND PRESSURE RESULTS AGREE TO WITHIN 0.5% (CALCULATED VS CONTAIN).
(2) COMPARISONS AMONG HB02, HB03, AND HB04 SHOW THAT PROBLEM TIME STEP HAS AN EFFECT ON CONTAIN RESULTS. TEST HB02 ESSENTIALLY USED A SINGLE TIME STEP ON THE SAME ORDER AS THE TOTAL H2 INJECTION PERIOD. IN THIS CASE THE CODE LOOKED AT THE CONDITIONS AT THE END OF THE TIME STEP. THESE CONDITIONS SATISFIED THE CRITERION FOR A COMPLETE H2 BURN (H2 CONCENTRATION IN EXCESS OF 10%). CONSEQUENTLY, ALL H2 WAS BURNED RATHER THAN BURNING DOWN TO 4% AS WAS INTENDED.

TEST HB04 USED A SMALLER TIME STEP THAN HB03, AND THE RESULTS SHOULD HAVE BEEN IDENTICAL TO HB03. INSTEAD, HB04 BURNED THE H2 DOWN TO A CONCENTRATION OF 3.86 MOLE %, WITH A CORRESPONDING TEMP AND PRESS OF 1383.8 K AND 5.1865E5 PA, RESPECTIVELY. THE DIFFERENCES BETWEEN HB03 AND HB04 ARE NOT LARGE, BUT THESE DIFFERENCES SHOULD NOT EXIST.

9. COMMENTS: OVERALL, CONTAIN APPEARS TO BE FOLLOWING THE PERSCRIBED BURN CRITERIA FAIRLY WELL. THE END STATE SYSTEM CONDITIONS AGREE WELL WITH PREDICTIONS BASED ON HAND CALCULATIONS. GROSS TIME STEPS COMPARED TO THE H2 SOURCE BEHAVIOR CAN LEAD TO ERRONEOUS RESULTS. TIME-STEP SIZE MUST BE CAREFULLY CHOSEN.

10. SUGGESTIONS FOR ADDITIONAL TESTS: CHECK CODE BEHAVIOR NEAR POINT OF TRANSITION FROM PARTIAL H2 BURN TO COMPLETE H2 BURN (10% H2 CONC.).

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1\. PROBLEM: ID NO. HB02,-4 2. LEVEL: PL2 3. RESOLVED? NO
4\. DESCRIPTION: RESULTS SOMEWHAT DEPENDENT ON TIME-STEP SIZE. GROSS TIME STEPS CAN LEAD TO USE OF IMPROPER BURN CRITERION.
5\. DATE PROBLEM RESOLVED:

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CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: HB05 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL2

3. TITLE OF TEST: TEST OF H2 AND O2 LIMITS FOR BURN CRITERIA

4. CODE VERSION (DATE): 208 (2/26/82)

5. ACTIVE MODULES OR OPTIONS: HYDROGEN BURN

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO HEAT STRUCTURES (ADIABATIC SYSTEM). CONTINUOUS INJECTION OF H2 AT A RATE OF 0.15 KG/S FOR A PERIOD OF 390 S.

7. TEST: (1) TEST INITIATION OF H2 BURN BASED ON H2 CONCENTRATION LIMITS WITH ADEQUATE O2 SUPPLY.
   (2) TEST TERMINATION OF H2-O2 REACTION AS O2 SUPPLY BECOMES DEPLETED.
   (3) TEST OVERALL QUALITATIVE BEHAVIOR.

8. RESULTS OF TEST: (1) H2 BURNING STARTED AS H2 CONCENTRATION EXCEEDED 4 MOLE %. THIS IS IN ACCORDANCE WITH LIMITING H2 CONCENTRATION FOR BURNING. (2) H2-O2 REACTION STOPPED WHEN THE O2 CONCENTRATION FELL TO 5 MOLE %. THIS IS IN ACCORDANCE WITH THE LIMITING O2 CONCENTRATION CRITERION. (3) QUALITATIVELY, THE CONTAIN RESULTS BEHAVE IN THE CORRECT MANNER. THE PRESSURE AND TEMPERATURE OF THE SYSTEM INITIALLY INCREASE SLOWLY AS A RESULT OF MASS BEING ADDED TO THE CONSTANT-VOLUME SYSTEM. ONCE THE H2 BURN CRITERION IS MET, THE ENERGY RELEASED BY THE H2-O2 REACTION RAPIDLY HEATS AND PRESSURIZES THE SYSTEM. THE H2 CONCENTRATION REMAINS AT 4 MOLE % DURING THIS PERIOD. BURNING CONTINUES UNTIL THE O2 CONCENTRATION FALLS TO 5 MOLE %, AT WHICH POINT IT STOPS. AT THIS POINT THE SYSTEM TEMPERATURE BEGINS TO DROP BECAUSE COLD H2 (TEMP = 298.0 K) CONTINUES TO FEED INTO THE SYSTEM. THE OVERALL SYSTEM PRESSURE, HOWEVER, CONTINUES TO INCREASE BECAUSE OF THE MASS BEING ADDED TO THE CONSTANT-VOLUME SYSTEM. TEMPERATURE AND PRESSURE CHANGES CEASE ONCE H2 INJECTION TERMINATES.

   FIGURES HB-02 THROUGH HB-06 SHOW THE SYSTEM RESPONSE VS TIME IN TERMS OF CELL TEMPERATURE, PRESSURE, H2 CONCENTRATION, O2 CONCENTRATION, AND H2O CONCENTRATION, RESPECTIVELY. THE JAGGED NATURE OF THE PLOTS, STARTING AT ABOUT 130 S, IS THE RESULT OF A CHANGE IN THE PROBLEM TIME-STEP SIZE. THE CHARACTERISTICS NOTED ABOVE ARE CLEARLY ILLUSTRATED IN THE PLOTS.

9. COMMENTS: CONTAIN APPEARS TO BE HANDLING H2 BURN PROBLEMS CORRECTLY. PLOTS OF H2 CONCENTRATION, TEMPERATURE, PRESSURE, ETC., CAN BE SOMEWHAT MISLEADING IN THAT THE PLOTTED VALUES ARE DEPENDENT ON THE PROBLEM TIME STEP. THE VALUES PLOTTED, AND THOSE IN THE LONG PRINT EDITS, REPRESENT THE SYSTEM CONDITIONS AT THE END OF THE TIME STEP BUT PRIOR TO THE OCCURRENCE OF ATMOSPHERE CHEMICAL REACTIONS FOR THAT TIME STEP. THEREFORE, THE LONGER THE TIME STEP

THE GREATER THE ACCUMULATION OF SOURCE MATERIALS FED IN DURING THAT TIME INTERVAL. CONTAIN PRINTOUTS AND PLOTS REFLECT THE QUANTITIES PRESENT IMMEDIATELY PRIOR TO THE CHEMICAL REACTIONS RATHER THAN THE CONDITIONS FOLLOWING THE REACTIONS. CARE MUST BE TAKEN TO ASSURE THAT THE TIME STEPS ARE APPROPRIATE FOR THE SOURCE RATES AND FOR THE LEVEL OF RESOLUTION DESIRED.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

1. PROBLEM: ID NO. HB05 2. LEVEL: PL1,PL2 3. RESOLVED? NO
4. DESCRIPTION: CONFUSION IN PLOT VALUES AND PRINTOUT VALUES FOR CERTAIN PARAMETERS IN THAT THEY ARE INFLUENCED BY PROBLEM TIME-STEP SIZE.
5. DATE PROBLEM RESOLVED:

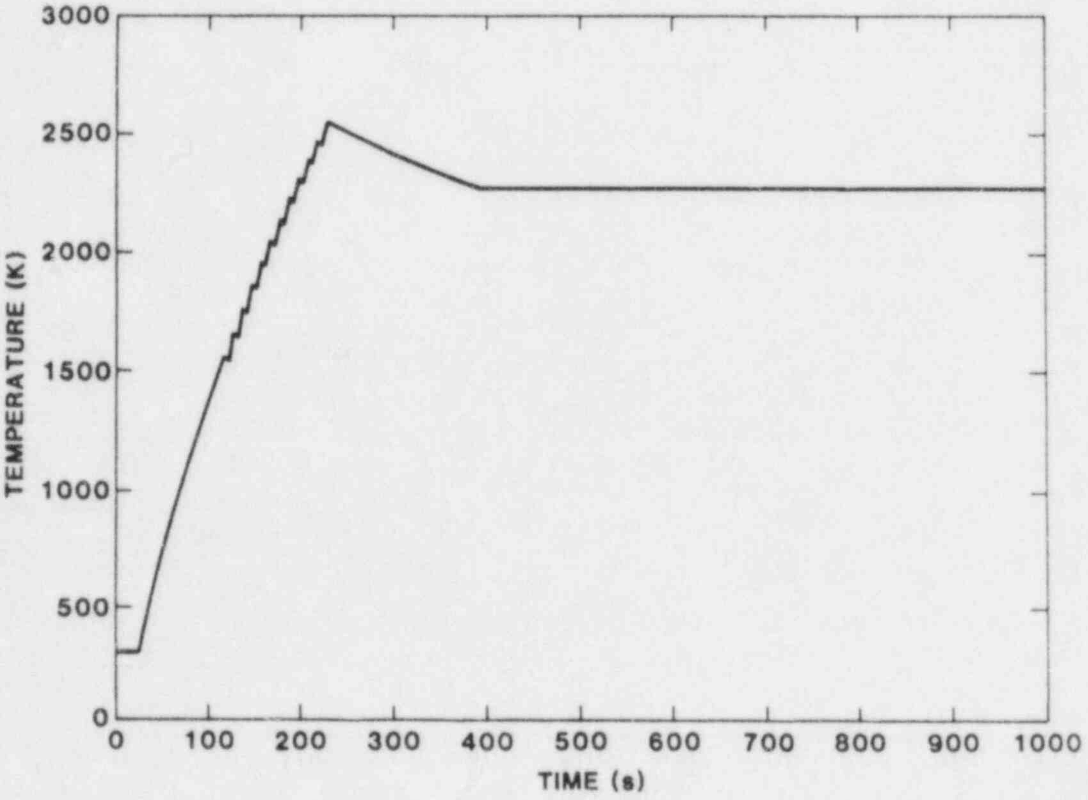

Figure HB-02 Cell gas temperature during hydrogen injection and burn (Test HB05).

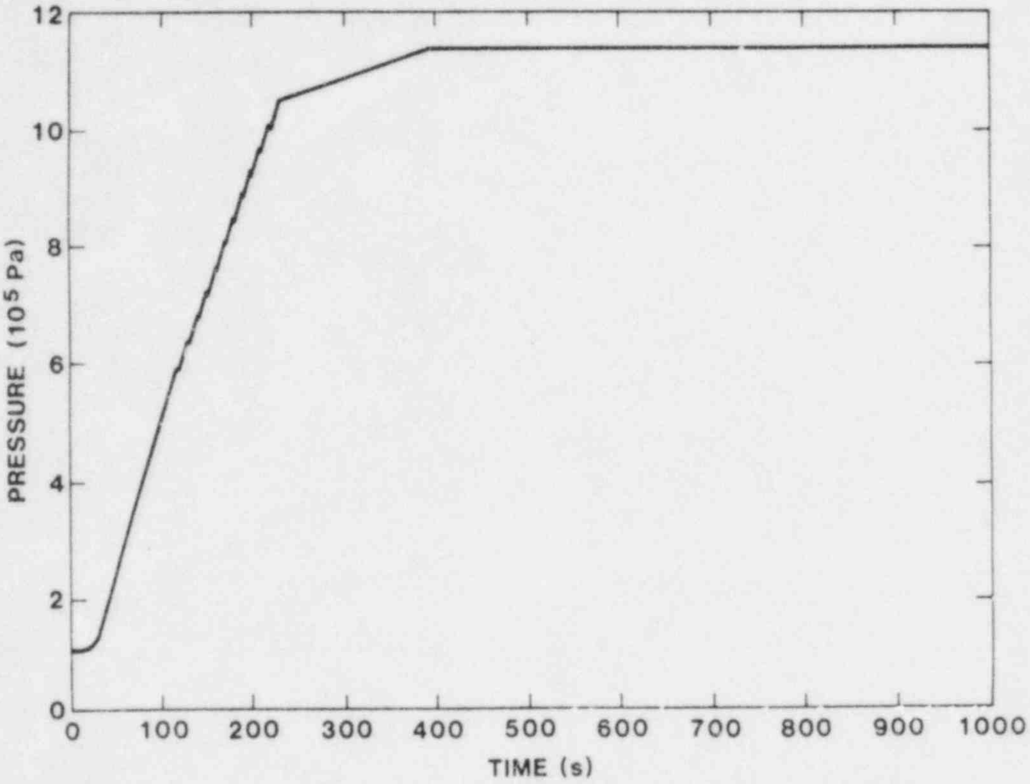

Figure HB-03 Cell pressure during hydrogen injection and burn (Test HB05).

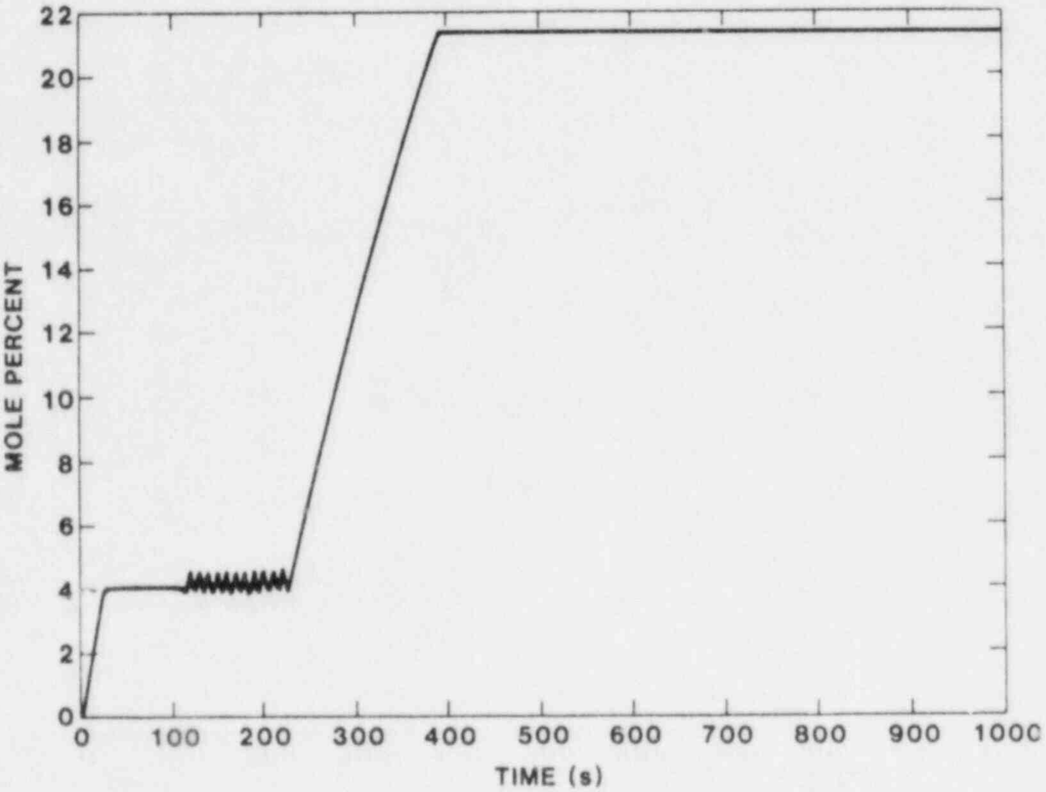

Figure HB-04 Hydrogen concentration during hydrogen injection and burn (Test HB05).

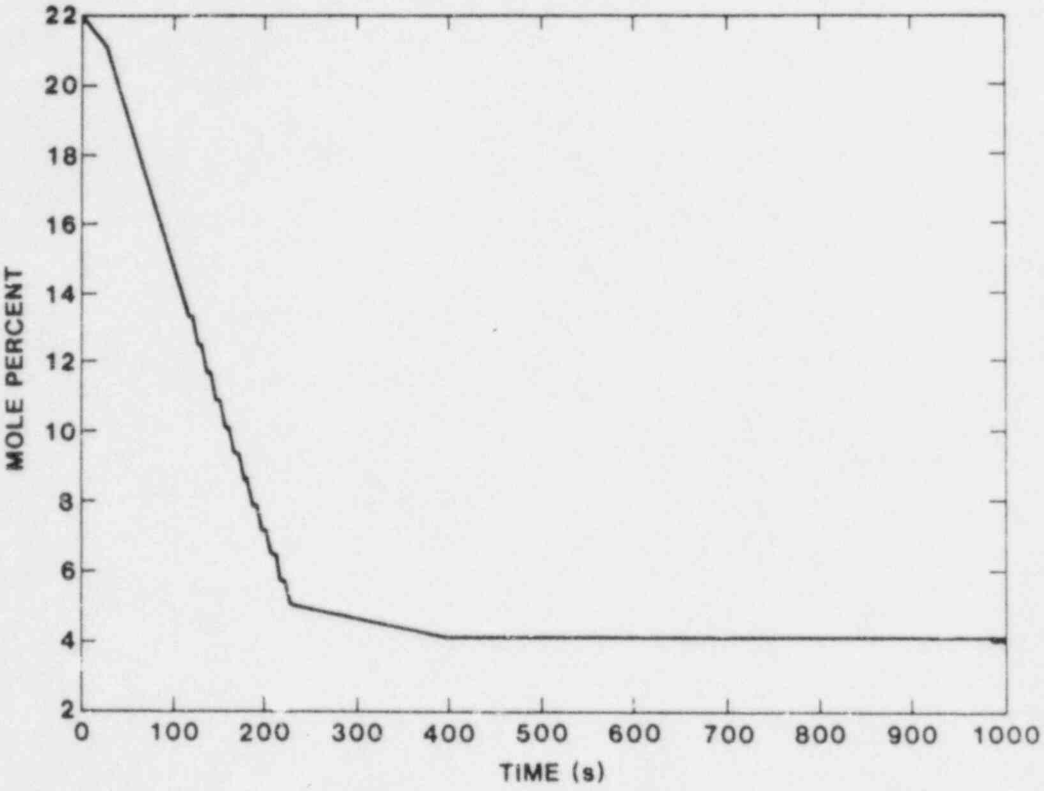

Figure HB-05 Oxygen concentration during hydrogen injection and burn (Test HB05).

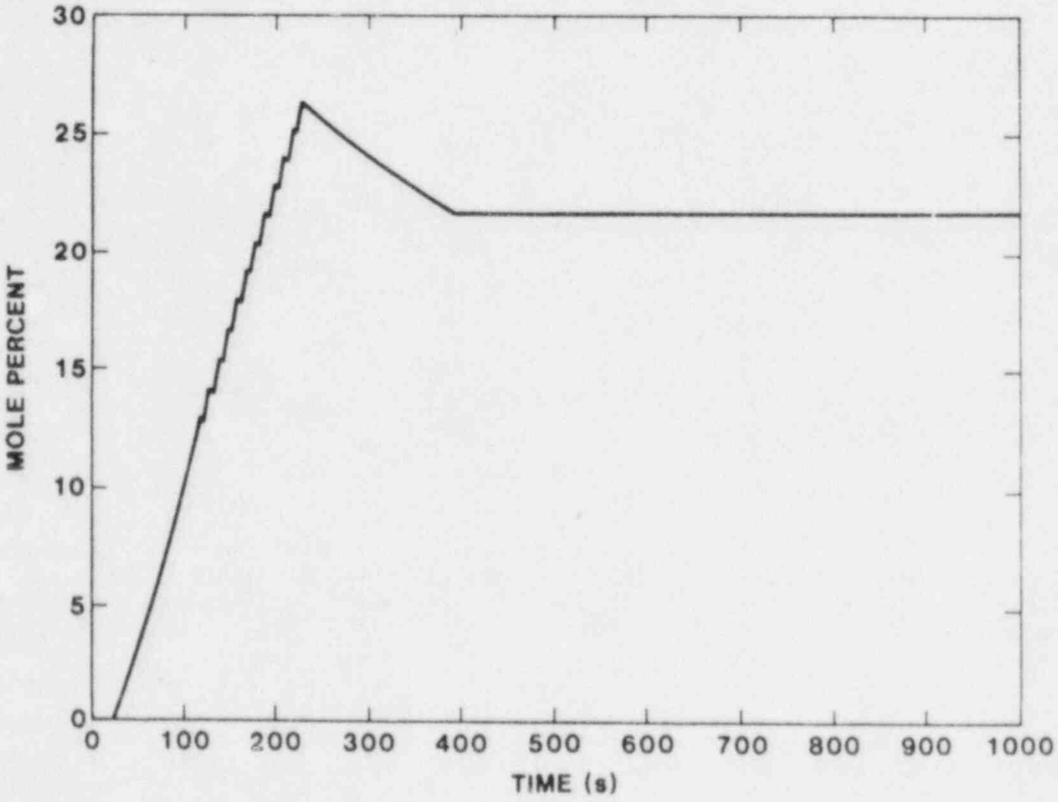

Figure HB-06 Water-vapor concentration during hydrogen injection and burn (Test HB05).

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: HB06 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL2

3. TITLE OF TEST: H2O-VAPOR SUPPRESSION OF HYDROGEN BURNS

4. CODE VERSION (DATE): 312 (3-18-82)

5. ACTIVE MODULES OR OPTIONS: HYDROGEN BURN, ATMOSPHERE THERMODYNAMICS

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO HEAT STRUCTURES. INITIAL ATMOSPHERE CONSISTS OF 30% O2, 70% H2O VAPOR, AT AMBIENT TEMPERATURE AND PRESSURE. CONTINUOUS INJECTION OF H2 FOR A PERIOD OF 390 S AT THE RATE OF 0.15 KG/S. INJECTION OF WATER VAPOR (600 K) STARTING AT 140 S FOR 40 S AT THE RATE OF 30 KG/S.

7. TEST: QUALITATIVE TEST OF H2O SUPPRESSION OF H2 BURN. ESTABLISH WHETHER CODE ALLOWS BURNS UNDER PROSCRIBED CONDITIONS.

8. RESULTS OF TEST: CONTAIN PREDICTED AN INSTANTANEOUS, NEARLY COMPLETE, BURN OF H2 AT THE POINT AT WHICH THE H2O VAPOR CONCENTRATION FELL TO 60%. THE O2 AND H2 CONCENTRATIONS AT THIS POINT WERE 25.7% AND 14.2%, RESPECTIVELY. BECAUSE OF THE LARGE BURN, THE WATER-VAPOR CONCENTRATION JUMPED FROM 60% TO 80%, SUPPRESSING ANY FURTHER H2-O2 REACTIONS. THIS BEHAVIOR IS ENTIRELY CONSISTENT WITH THE BURN CRITERIA ESTABLISHED FOR HYDROGEN BURNS. TEMPERATURE AND PRESSURE BEHAVIOR WERE AS EXPECTED FOR THE PROBLEM CONDITIONS.

9. COMMENTS: CONTAIN APPEARS TO BE HANDLING H2O SUPPRESSION OF H2 BURNS IN THE CORRECT MANNER.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

Supporting Analysis: HB Series - Hydrogen Burns

In this test series, hydrogen is introduced into an air-filled cell. Hydrogen reacts with oxygen to produce water.

$$1.0\ H_2 + 0.5\ O_2 \dashrightarrow 1.0\ H_2O \qquad (3.2\text{-}1)$$

The objective is to predict the end-state conditions in an adiabatic, air-filled cell following either a complete or partial hydrogen burn.

Assume that the end state is reached in two stages. The burn is a constant-volume process, so internal energy is used rather than enthalpy. In the first stage

$$\text{Reactants } (T_1) \dashrightarrow \text{Products } (T_1) \qquad (3.2\text{-}2)$$

for which

$$\Delta U_1 = -Q_v = U_{prod} - U_{reactants} \qquad (3.2\text{-}3)$$

where

ΔU_1 = change in internal energy accompanying the reaction at T_1

U_{prod} = Internal energy of reaction products at temp T_1

$U_{reactants}$ = Internal energy of reactants at temp T_1

In the second stage

$$\text{Products } (T_1) \dashrightarrow \text{Products } (T_2) \qquad (3.2\text{-}4)$$

and ΔU_2, representing the change in internal energy in raising the products from T_1 to T_2, is given by

$$\Delta U_2 = \int_{T_1}^{T_2} \eta C_v(\text{Prod})dT \qquad (3.2\text{-}5)$$

where η = number of moles and C_v(Prod) = specific heat at constant volume of reaction products.

Because the system is adiabatic, the internal energy of reaction is equal to the internal energy of the products:

$$\Delta U_1 = -\Delta U_2 = -\int_{T_1}^{T_2} \eta C_v(\text{Prod})dT \qquad (3.2\text{-}6)$$

For this system, products consist of all components present at the end state, so

$$\int_{T_1}^{T_2} \eta C_v(\text{Prod})dT = \int_{T_1}^{T_2} (\eta C_v)_{H_2O} dT + \int_{T_1}^{T_2} (\eta C_v)_{N_2} dT$$

$$+ \int_{T_1}^{T_2} (\eta C_v)_{O_2} dT + \int_{T_1}^{T_2} (\eta C_v)_{H_2} dT \qquad (3.2\text{-}7)$$

In the computations used here, C_v is expressed as a function of temperature for each component in the cell. The functional form is

$$C_{v_i} = a_i + b_i T + c_i T^2 \qquad (3.2\text{-}8)$$

Thus, the known reaction energy can be equated to a function of temperature, and the end-state temperature T_2 can then be determined.

SERIES HB STANDARD TEST INPUT DATA SET

```
&&-------------------------- CASE HB03(ST) -----------------------------
CONTROL=9 1 3 3 4 2 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL
H2O H2OV H2OL
FISSION
TE132 I132
I133 XE133
TIMES 50.0 0.0 1.0 1.0 40.0 5.0 5.0 1.0E2 1.0E2 5.0E2 1.0E3 1.0
FLOWS
PRFISS
PRH-BURN
FISSION 0 2 2
TE132 I132
I133 XE133
1.0E5 2.0E5
1.0E5 1.0E6
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 1.0 1.0
EOI
TITLE
               HYDROGEN BURN TESTS
  CASE HB03(ST):  CONTINUOUS INJECTION OF H2 INTO AIR FILLED CELL
      TEST BURN CRITERION AND TEMP INCREASE (ADIABATIC CELL)
FAST
CELL =1
CONTROL=18 0 0 0 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0
H-BURN
GEOMETRY 1128.52 10.0
ATMOS=2
1.013E5  298.0
N2=0.7800
O2=0.22
&&  -------15 KG OF HYDROGEN INJECTED INTO CELL IN 100 SECONDS-----------
SOURCE=1
H2=2
IFLAG=1
T=0.0 100.0
MASS=0.15 0.0
TEMP=298.0 298.0
EOI
EOF
```

3.2.2 Series SB - Sodium-Vapor Combustion and Na_2O/H_2O Reactions

Tests SB01 and SB02 exercised CONTAIN's treatment of sodium-vapor/air chemistry. In these tests sodium vapor was injected into an air-filled cell, allowing the sodium and oxygen to react chemically. This reaction forms Na_2O, which can subsequently react with water or water vapor to form NaOH. Test SB03 tested the second reaction.

These tests revealed that CONTAIN is handling these atmosphere chemical reactions as intended. The CONTAIN results were in good agreement with those obtained from the check calculations. However, the current CONTAIN coding is based on the assumption that all chemical heating from reactions taking place in the atmosphere is absorbed only by the gases present. This is a conservative assumption, i.e., higher atmosphere temperatures and pressures are produced than would be the case were some of the chemically produced heat absorbed by the solids or liquids produced by the reactions.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: SB01 AND SB02(ST) USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A

3. TITLE OF TEST: COMBUSTION OF SODIUM VAPOR

4. CODE VERSION (DATE): 312 (3-29 AND 4-6-82)

5. ACTIVE MODULES OR OPTIONS: ATMOSPHERE CHEMISTRY AND ATMOSPHERE THERMODYNAMICS

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE AIR-FILLED CELL WITH NO HEAT SINKS (ADIABATIC SYSTEM). INITIAL TEMPERATURE AND PRESSURE WERE 298 K AND 1.0E5 PA. THE CELL VOLUME WAS SIZED TO ACCOMMODATE 100 KG-MOLES OF GAS AT THESE CONDITIONS.
   (1) FOR TEST SB01 2.5 KG-MOLES (57.475 KG) OF SODIUM VAPOR AT A TEMPERATURE OF 298 K WERE INJECTED INTO THE CELL OVER A TEN-SECOND SPAN.
   (2) FOR TEST SB02 THE QUANTITY OF SODIUM VAPOR WAS INCREASED TO 6.0 KG-MOLES TO TEST THE EFFECT OF CERTAIN ASSUMPTIONS IN CONTAIN. ALL ELSE WAS THE SAME AS FOR TEST SB01.

7. TEST: HAND CALCULATIONS WERE MADE TO PREDICT THE FINAL TEMPERATURE AND PRESSURE CONDITIONS FOR THE SYSTEM. ALL OF THE SODIUM VAPOR WAS ASSUMED TO REACT WITH THE OXYGEN TO FORM NA2O. TWO CASES WERE EXPLORED: (1) ALL CHEMICAL HEATING WAS ASSUMED TO BE ABSORBED BY THE GASES PRESENT AT THE TERMINATION OF THE REACTION, OR (2) THE NA2O FORMED WAS ALSO ASSUMED TO BE AT THE FINAL EQUILIBRIUM TEMPERATURE. THE RESULTS OF THE HAND CALCULATIONS WERE THEN COMPARED TO THE CONTAIN RESULTS.

8. RESULTS OF TEST: THE FOLLOWING TABLE GIVES THE KEY CONTAIN RESULTS AND COMPARES THEM WITH RESULTS FROM THE HAND CALCULATIONS.

CASE SB01:	TEMP, K	PRESS, 1.E5 PA
CONTAIN RESULTS	666.7	2.223
CALCULATIONS(NA2O EXCL)	661.2	2.207
CALCULATIONS(NA2O INCL)	643.7	2.146
CASE SB02:		
CONTAIN RESULTS	1142.0	3.775
CALCULATIONS(NA2O EXCL)	1139.3	3.766
CALCULATIONS(NA2O INCL)	1055.4	3.488

THE CODING IN CONTAIN IS BASED ON THE ASSUMPTION THAT ALL CHEMICAL HEAT PRODUCED BY REACTIONS TAKING PLACE IN THE ATMOSPHERE IS ABSORBED ONLY BY THE GASES PRESENT. THE CONTAIN RESULTS AGREE VERY CLOSELY WITH THE RESULTS OF HAND CALCULATIONS BASED ON THE SAME ASSUMPTION. FOR EXAMPLE, THE DIFFERENCE IN THE PREDICTED FINAL TEMPERATURES IS LESS THAN 1% FOR SB01 AND ONLY ABOUT 0.3% FOR SB02. BASED ON THE ASSUMPTION USED, CONTAIN RESULTS FOR SODIUM-VAPOR BURNS ARE SATISFACTORY.

9. COMMENTS: THE ASSUMPTION THAT THE GASES IN THE ATMOSPHERE ABSORB ALL OF THE HEAT FROM ATMOSPHERIC REACTIONS LEADS TO OVERESTIMATES OF THE ACTUAL END-STATE TEMPERATURES AND PRESSURES. THEREFORE, THESE ESTIMATES ARE PROBABLY CONSERVATIVE FOR MOST CASES. A MORE REALISTIC ASSUMPTION WOULD BE THAT SOME OF THE REACTION HEAT IS ABSORBED BY SOME OF THE SOLID OR LIQUID REACTION PRODUCTS.

   NOTE THAT THE CURRENT CONTAIN CODING DOES NOT ALLOW FOR BURNING OF LIQUID SODIUM IN THE ATMOSPHERE UNLESS THE SPRAY-FIRE OPTION IS INVOKED.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

1. PROBLEM: ID NO. SB01-01 2. LEVEL: PL2 3. RESOLVED? NO
4. DESCRIPTION: FOR ATMOSPHERE CHEMICAL REACTIONS THE CHEMICAL HEATING IS ABSORBED ONLY BY THE ATMOSPHERIC GASES; LIQUIDS OR SOLIDS FORMED BY THE REACTIONS ARE IGNORED IN DETERMINING THE SYSTEM THERMAL CONDITIONS.
5. DATE PROBLEM RESOLVED:

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: SB03 USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: REACTION OF NA2O WITH H2O TO FORM NAOH
4. CODE VERSION (DATE): 312 (4-22-82)
5. ACTIVE MODULES OR OPTIONS: ATMOSPHERE CHEMISTRY AND THERMODYNAMICS

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE ADIABATIC CELL SIZED TO CONTAIN 100 KG-MOLES OF GAS INITIALLY AT AMBIENT PRESSURE AND TEMPERATURE (1.0E5 PA AND 298 K). CELL WAS INITIALLY FILLED WITH H_2O VAPOR. NO HEAT STRUCTURES PRESENT. NA_2O WAS THEN INTRODUCED AS A SOURCE WITH INPUT RATE OF 30.99 KG/S FOR A PERIOD OF 10 S (TOTAL QUANTITY WAS 309.9 KG). THE NA_2O WAS AT AN INITIAL TEMPERATURE OF 298 K.

7. TEST: HAND CALCULATIONS WERE MADE TO PREDICT THE FINAL TEMPERATURE AND PRESSURE CONDITIONS FOR THE SYSTEM. ALL OF THE NA_2O WAS ASSUMED TO REACT WITH THE WATER VAPOR PRESENT. AS WITH TESTS SB01 AND SB02, TWO CASES WERE EXPLORED: (1) ALL CHEMICAL HEATING WAS ASSUMED TO BE ABSORBED BY THE GASES PRESENT AT THE TERMINATION OF THE REACTION, OR (2) THE NAOH FORMED IN THE REACTION WAS ALSO ASSUMED TO BE AT THE FINAL EQUILIBRIUM TEMPERATURE. THE RESULTS OF THE HAND CALCULATIONS WERE THEN COMPARED WITH THE CONTAIN RESULTS.

8. RESULTS OF TEST: RESULTS FROM HAND CALCULATIONS AND THOSE FROM CONTAIN WERE IN GOOD AGREEMENT FOR THE CASE (1) ASSUMPTION NOTED ABOVE. THE END-STATE CONDITIONS PREDICTED ARE AS FOLLOWS:

	TEMP, K	PRESS, 1.0E5 PA
CONTAIN RESULTS	674.5	2.150
CALCULATIONS(NAOH EXCLUDED)	673.4	2.147
CALCULATIONS(NAOH INCLUDED)	570.0	1.817

IN CONTAIN'S TREATMENT AND IN THE HAND CALCULATIONS ALL OF THE NA_2O INJECTED INTO THE SYSTEM WAS ALLOWED TO REACT.

9. COMMENTS: THE NUMBERS IN THE FOREGOING TABLE INDICATE THE SENSITIVITY OF THE FINAL CONDITIONS TO THE ASSUMPTION THAT ALL OF THE REACTION PRODUCTS ARE IN THERMAL EQUILIBRIUM. FOR THIS PARTICULAR PROBLEM ONLY 5 KG-MOLES OF NA_2O WERE REACTED WITH 100 KG-MOLES OF H_2O. AS IS APPARENT, A SMALL QUANTITY OF SOLID PRODUCTS (10 KG-MOLES OF NAOH), CAN HAVE A LARGE EFFECT ON THE END STATE OF THE SYSTEM WHEN THESE SOLIDS ARE INCLUDED IN THE FINAL ENERGY BALANCE. THE CONTAIN PREDICTIONS OF SYSTEM TEMPERATURE AND PRESSURE ARE PROBABLY CONSERVATIVE FOR MOST CASES.

THE RESULTS OBTAINED WERE GENERATED WITH THE "FAST" REACTOR OPTION OF THE CODE. THE "THERMAL" REACTOR OPTION DOES NOT ALLOW THE NA_2O/H_2O REACTION.

10. SUGGESTIONS FOR ADDITIONAL TESTS: CHECK MORE COMPLEX CHEMICAL SYSTEMS SUCH AS THOSE RESULTING FROM THE INJECTION OF NA VAPOR INTO AN ATMOSPHERE CONTAINING O_2 AND H_2O.

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1. PROBLEM: ID NO. SB03-01 2. LEVEL: PL2 3. RESOLVED? NO
4. DESCRIPTION: FOR ATMOSPHERE CHEMICAL REACTIONS THE CHEMICAL HEATING IS ABSORBED ONLY BY THE ATMOSPHERIC GASES, AND LIQUIDS OR SOLIDS FORMED BY THE REACTIONS ARE IGNORED IN DETERMINING THE SYSTEM THERMAL CONDITIONS.
5. DATE PROBLEM RESOLVED:

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Supporting Analysis: SB Series - Sodium-Vapor Combustion and Na_2O/H_2O Reactions

A. Combustion of Sodium Vapor:

Note: The symbol usage below is consistent with the usage and definitions presented in the supporting analysis for the HB Series of tests.

Sodium vapor is injected into an adiabatic, air-filled cell. Calculate the end-state conditions following the combustion of the injected sodium.

The reaction equation is

$$\eta_{N_2} N_2 + \eta_{O_2} O_2 + \eta_{Na} Na \dashrightarrow \eta_{N_2} N_2 + \frac{\eta_{Na}}{2} Na_2O + (\eta_{O_2} - \frac{\eta_{Na}}{4}) O_2 \qquad (3.2\text{-}9)$$

Assume that the chemical reaction proceeds in two stages. It is a constant-volume process, so the energy balance is based on internal energies. In the first stage

$$\text{Reactants } (T_1) \dashrightarrow \text{Products } (T_1) \qquad (3.2\text{-}2)$$

with an accompanying change in internal energy ΔU_1 due to the reaction at constant temperature T_1. In the second stage

$$\text{Products } (T_1) \dashrightarrow \text{Products } (T_2) \qquad (3.2\text{-}4)$$

where ΔU_2 is the change in internal energy associated with raising the temperature of the products from T_1 to T_2.

Since the system is adiabatic, there is no net gain or loss of energy in the system, i.e.,

$$\Delta U_1 + \Delta U_2 = 0 \qquad (3.2\text{-}10)$$

or

$$\Delta U_1 = -\Delta U_2 \qquad (3.2\text{-}11)$$

Note that $H = U + pV$.

For gaseous reactants and products

$$pV = \eta RT \qquad (3.2\text{-}12)$$

Therefore,

$$H = U + pV = U + \eta RT \qquad (3.2\text{-}13)$$

The change in internal energy that takes place during the reaction at temperature T can be determined from the change in enthalpy

$$\Delta H_T = H_{prod} - H_{reac} = U_p + \eta_p RT - (U_r + \eta_r RT) \qquad (3.2\text{-}14)$$

or

$$\Delta H_T = U_p - U_r + (\eta_p - \eta_r)RT = \Delta U_T + \Delta\eta_g RT \qquad (3.2\text{-}15)$$

where $\Delta\eta_g$ is the difference between the number of moles of <u>gaseous</u> reaction products and the number of moles of <u>gaseous</u> reactants.

The change in internal energy brought about by the reaction at T_1 is therefore

$$\Delta U_1 = \Delta H_1 - \Delta\eta_g RT_1 \qquad (3.2\text{-}16)$$

Thus, ΔU_1 can be calculated from the enthalpies of the products and reactants and the change in the number of moles of gas in the system.

To find the end-state conditions (at $T = T_2$), ΔU_1 is set equal to $-\Delta U_2$ where

$$\Delta U_2 = \sum_{i=1}^{N} \left[\eta_i u_i(T_2) - \eta_i u_i(T_1)\right]\text{prod} \qquad (3.2\text{-}17)$$

and N refers to all products. For products other than gaseous products, $u_i = h_i$; for gaseous products, $u_i = h_i - RT$, and

$$\Delta U_2 = \sum_{i=1}^{N} \eta_i\left[h_i(T_2) - h_i(T_1)\right] - \sum_{k=1}^{N(g)} \eta_{k(g)} R(T_2 - T_1) \qquad (3.2\text{-}18)$$

where $N_{(g)}$ refers to gaseous products only. Consequently,

$$\begin{aligned}\Delta U_2 &= \eta_{N_2}\left[h_{N_2}(T_2) - h_{N_2}(T_1) - R(T_2 - T_1)\right] \\ &+ \eta_{O_2}\left[h_{O_2}(T_2) - h_{O_2}(T_1) - R(T_2 - T_1)\right] \\ &+ \eta_{Na_2O}\left[h_{Na_2O}(T_2) - h_{Na_2O}(T_1)\right]\end{aligned} \qquad (3.2\text{-}19)$$

A trial and error solution is used to find the final temperature, T_2, of the system.

The above analysis does not explicitly account for the fact that as sodium is injected into the system it does some flow work. Therefore, the enthalpy of the injected sodium should be used rather than its internal energy. If the flow work is included, it makes a slight difference in the calculated end-state temperature.

B. Reaction of Na_2O with H_2O to Form NaOH:

The assumed chemical reaction is

$$1.0\ Na_2O + 1.0\ H_2O \dashrightarrow 2.0\ NaOH \qquad (3.2\text{-}20)$$

For excess amounts of H_2O:

$$(\eta_{Na_2O})Na_2O + (\eta_{H_2O})H_2O \dashrightarrow (2\eta_{Na_2O})NaOH + (\eta_{H_2O} - \eta_{Na_2O})H_2O \quad (3.2\text{-}21)$$

For this problem Na_2O is injected into a cell filled with H_2O vapor. The reaction process takes place at constant volume in an adiabatic cell.

As in the previous analysis, the reaction can be assumed to proceed in two stages, and the end-state temperature can be determined by the same procedure used in the analysis of the combustion of sodium vapor.

SERIES SB STANDARD TEST INPUT DATA SET

```
&&      -------------SB02(ST) DATA FILE ------------------

CONTROL=9 1 3 1 4 2 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL NA2O
H2O H2OV H2OL
FISSION
TE132 I132
I133 XE133
TIMES 50.0 0.0 1.0 1.0 40.00 1.0
FLOWS
FISSION 0 2 2
TE132 I132
I133 XE133
1.0E5 2.0E5
1.0E5 1.0E6
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 1.0 1.0
EOI
TITLE
                      SODIUM BURNS IN ATMOSPHERE TESTS
   CASE SB02:  INJECTION OF 6.0 KG-MOLES (137.940 KG) OF SODIUM INTO
       AIR FILLED CELL.  NO HEAT STRUCTURES, ADIABATIC SYSTEM.
FAST
CELL =1
CONTROL=18 0 0 0 0 0 0 1 2 0 0 0 0 0 0 0 0 0 0
GEOMETRY 2477.66 10.0
ATMOS=2
1.000E5  298.0
N2=0.7800
O2=0.22
&&      ------ INJECTION OF NAV; 57.475 KG IN 10 SECONDS ------------------
SOURCE=1
NAV=2
IFLAG=1
T=20.0 30.0
MASS=13.794 0.0
TEMP=298.0 298.0
EOI
ATMCHEM
EOF
```

3.2.3 Series SF - Sodium-Spray Fires

Sodium-spray fires are of concern in LMFBRs because they have the potential for causing rapid and substantial temperature and pressure increases. This test series checked CONTAIN's treatment of this phenomenon. The test results show that CONTAIN gives good predictions of the conditions following a sodium-spray fire.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: SF01(ST) THRU SF05 USER NAME: P. REXROTH
2. TEST LEVEL: TL4C
3. TITLE OF TEST: SODIUM-SPRAY FIRE: COMPARISON WITH NACOM CODE
4. CODE VERSION (DATE): 1B-03-82 MOD000 (4/16/82)
5. ACTIVE MODULES OR OPTIONS: SPRAY FIRE, STRUCTURE H.T., AEROSOLS
6. CONTAINMENT CONFIGURATION AND SOURCES: ONE CELL INITIALLY AT 1.E5 PA AND 297 K. INITIAL ATMOSPHERES VARIED FROM .5% TO 20% OXYGEN. CONSTANT 1 KG/S SOURCE OF SODIUM SPRAY AT 811 K FOR 3 S.
7. TEST: COMPARE THE CALCULATED MASS OF SODIUM BURNED AND THE RESULTING HEAT TRANSFERRED TO THE ATMOSPHERE TO THAT CALCULATED BY THE NACOM COMPUTER CODE. INITIAL ATMOSPHERIC OXYGEN MOLAR PERCENTAGES ARE 0.5% (SF01), 1.0% (SF02), 5.0% (SF03), 10.0% (SF04), AND 20.0% (SF05). THE CELL GEOMETRY AND HEAT-TRANSFER SURFACES ARE SIMILAR TO THOSE USED IN ATOMICS INTERNATIONAL'S JET TEST SERIES. NACOM'S PREDICTIONS HAVE BEEN CORROBORATED IN THE AI TESTS.
8. RESULTS OF TEST: (1) FOR THE FIVE TESTS, THE CONTAIN VALUES OF MASS OF SODIUM BURNED VARIED FROM AN UNDERPREDICTION OF 15% (SF03) TO AN OVERPREDICTION OF 9% (SF04) AS COMPARED TO THE NACOM VALUES. (2) VALUES FOR THE QUANTITY OF HEAT TRANSFERED TO THE ATMOSPHERE VARIED FROM AN UNDERPREDICTION OF 6% (SF01) TO AN OVERPREDICTION OF 13% (SF04) AS COMPARED WITH THE NACOM RESULTS.
9. COMMENTS: THE AGREEMENT BETWEEN CONTAIN AND NACOM WAS SATISFACTORY CONSIDERING THE UNCERTAINTIES AND SIMPLIFICATIONS INHERENT IN EACH MODEL. DIFFERENCES IN DROPLET-TO-ATMOSPHERE HEAT TRANSFER, ATMOSPHERE-TO-WALL HEAT TRANSFER, AND MATERIAL PROPERTIES HAVE BEEN SHOWN TO BE RESPONSIBLE FOR SOME OF THE DISPARITY BETWEEN THE TWO CODES.
10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

==

1. PROBLEM: ID NO.SF01-01 2. LEVEL: PL1 3. RESOLVED? NO
4. DESCRIPTION: SODIUM-SPRAY SOURCE-TABLE INTERPRETATION ERROR. THE SOURCE WAS TO BE TERMINATED AT 3 S. IF A VALUE OF 3.0 IS INPUT, THE SOURCE DOES NOT TERMINATE UNTIL THE NEXT TIME STEP, I.E., 3.5 S. FOR THIS TEST AN INJECTION TIME OF 2.999 S SHOULD BE USED TO ENSURE TERMINATION AT 3 S.
5. DATE PROBLEM RESOLVED:

==

Supporting Analysis: SF Series - Sodium-Spray Fires

The sodium-spray-fire model in CONTAIN is based on the oxidation and combustion equations and the droplet-size distribution used in the NACOM (Ref. 1) computer code. Alternative droplet dynamics and numerical solution schemes were, however, developed for CONTAIN. Because NACOM has been tested and accepted, comparisons of CONTAIN's results with NACOM's results were used to evaluate the performance of CONTAIN.

Because the oxidation chemistry of sodium is sensitive to the amount of oxygen available, the molar percentage of oxygen was used as the variable parameter in this series of test problems. Five test problems were run in which the oxygen molar percentages were varied from 0.5% to 20%. The geometry used for the calculations was similar to that used in Atomics International's Jet test series. This series provided the data used in confirming the NACOM computations. The vessel used by AI (and therefore the cell used in CONTAIN) was approximately 10 meters high, with a volume of 62 cubic meters. For all test problems, a sodium injection rate of 1 kg/s was maintained for 3 seconds.

For each problem, the rate of sodium combustion and the amount of heat transferred to the atmosphere were compared to corresponding quantities calculated using NACOM. The results of the comparison for the 20%-oxygen case are shown in Figure SF-01. The difference in the shapes of the CONTAIN and NACOM curves reflects the fact that NACOM solves the transient equation of motion of each droplet, whereas CONTAIN assumes that each droplet falls at its terminal velocity. The NACOM treatment provides resolution (1) during the time intervals following the start of the spray, in which the concentration of droplets in the atmosphere approaches a steady state, and (2) during the time interval following the termination of the spray, in which fallout of the droplets occurs. Calculated values of the total sodium burned and of the total heat transferred to the atmosphere are nearly identical for the two codes.

REFERENCE

1. S. S. Tsai, The NACOM Code for Analysis of Postulated Sodium Spray fires in LMFBRs, Brookhaven National Laboratory report NUREG/CR-1405, BNL-NUREG-51180, March 1980.

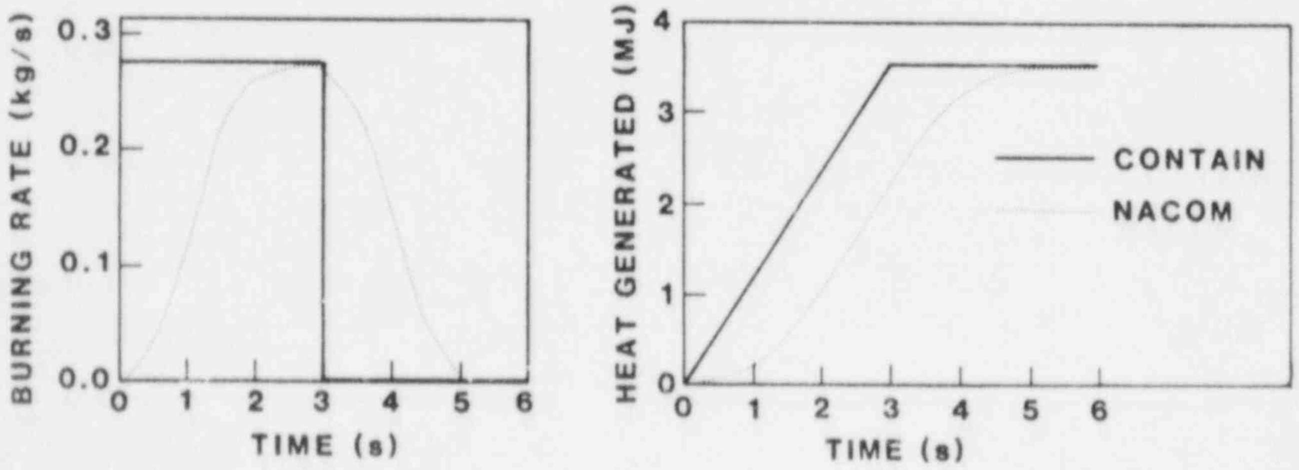

Figure SF-01 Comparison of CONTAIN and NACOM calculations for a sodium-spray fire.

SERIES SF STANDARD TEST INPUT DATA SET

```
&&      ---------- TEST SF01(ST) ------------------------------------ ----

CONTROL=9 1 1 1 2 1 20 2 0 0
&& TEST APPROXIMATES CONDITIONS IN AI JET8 TEST
MATERIAL
COMPOUND N2 NA O2 NA2O NA2O2 NAOH FE SIO3
FISSION DUM1 DUM2
TIMES 60. 0. 0.5 0.5 5.0 1.
FISSION
0 2
DUM1 DUM2
1.0E8 1.0E10
2*2.5E4 EOI
PRAER
PRSPRAY
PRHEAT
TITLE
NACOM-CONTAIN COMPARISON  SF01(ST)  0.5% O2
FAST
FLOWS
AEROSOL 0. 0. 0. 0. 0. 0. 0.  NA2O 0. 0. NA2O2 0. 0.
CELL=1
CONTROL=18 0 0 1 10 0 0 0 0 1 8 0 0 0 0 0 0 0 0
GEOMETRY 62.2971 10.0
ATMOS=2
1.0000E5 297.
N2=.995 O2=.005
STRUC VESSEL WALL SLAB 10 2 297. 1. 0. 297. 93.59
&& STRUCTURE SIMULATES AI JET EXPERIMENTAL VESSEL
0.0 0.001 0.003 0.0066 0.014 0.040 0.070 0.1 0.2 0.4 0.8
FE FE FE SIO3 N2 N2 N2 N2 N2 N2
SPRAFIRE 10.0 4.0E-3 0.0
SOURCE=1
NAL=2
IFLAG=1
T=0. 3.0
MASS=1.0 1.0
TEMP=811. 811.
EOF
```

3.3 INTERCELL-FLOW TESTS

3.3.1 Series CF - Intercell Flow of Gases

CONTAIN provides users with two options for modeling the flow of gases from one cell to another. One model employs a quasi-steady-state formulation for flows. This is a simple model, but it gives good results for a great many applications. The second model employs a more rigorous formulation for flow. It contains an inertial term, which provides for more realistic treatment of rapidly changing flow conditions. This test series tested both of these flow options.

Tests CF01, CF02, and CF04 used the quasi-steady-state flow model. The CONTAIN runs, and the supporting hand analysis used to check the CONTAIN results, simulated an isothermal blowdown between two cells. Test CF05 modeled the same system but employed the more rigorous flow-model option in the code. The results from all of these tests indicated that CONTAIN's treatment of isothermal flow was quite good. The results also indicated that if the flow routine with the inertial term is used, the time steps for the problem must be chosen very carefully; otherwise, some problems with convergence may occur.

Tests CF06 and CF07 exercised the inertial flow option and the quasi-steady-state option, respectively, to simulate an adiabatic blowdown between two cells. As with the other tests in this series, the CONTAIN results appear to be quite good.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: CF01, CF02, & CF04(ST) USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: INTERCELL FLOW - QUASI-STEADY-STATE MODEL
4. CODE VERSION (DATE): 308 (3-9,10-82)
5. ACTIVE MODULES OR OPTIONS: QUASI-STEADY-STATE FLOW ROUTINE, ATMOSPHERE THERMODYNAMICS
6. CONTAINMENT CONFIGURATION AND SOURCES: TWO EQUAL VOLUME CELLS, CELL #1 WITH AN INITIAL PRESSURE OF 1.1E5 PA AND CELL #2 WITH AN INITIAL PRESSURE OF 1.0E5 PA; EACH CELL WAS INITIALLY AT 300 K.
   (1) TEST CF01 REPRESENTED A FIRST ATTEMPT TO SIMULATE ISOTHERMAL CONDITIONS. A FLOW AREA OF 0.05 SQ M WAS USED. (2) TESTS CF02 AND CF04 EMPLOYED LARGE HEAT SINKS TO MAINTAIN THE GAS TEMPERATURE NEARLY ISOTHERMAL. THE FLOW AREA USED IN THESE CASES WAS 0.005 SQ M. THE CELLS WERE FILLED WITH HYDROGEN GAS. NO OTHER SINKS OR SOURCES WERE USED.
7. TEST: COMPARE AS A FUNCTION OF TIME THE INTERCELL FLOW RATE, THE CELL PRESSURES, AND THE CELL MASSES CALCULATED BY CONTAIN AND THOSE DERIVED FROM A SEPARATE HAND ANALYSIS. THE SEPARATE HAND ANALYSIS USED THE SAME BASIC QUASI-STEADY-FLOW MODEL AS CONTAIN DID BUT ASSUMED ISOTHERMAL CONDITIONS. IT ALSO GAVE A SPECIFIC FORMULATION OF THE KEY PARAMETERS AS A FUNCTION OF TIME.

8. RESULTS OF TEST: (1) CF01 COMPARED THE ISOTHERMAL CASE FROM HAND CALCULATIONS WITH THE CONDITIONS USED IN THE CONTAIN ANALYSIS. THE CONTAIN GAS TEMPERATURES DEVIATED FROM THE ISOTHERMAL CASE BY +/- 8 K. THE PREDICTED FLOW FROM CONTAIN DIFFERED FROM THAT OF THE HAND ANALYSIS BY ABOUT 30% OVER MOST OF THE FLOW RANGE, AND BY A FACTOR OF 2 OR MORE AT LOW FLOW RATES. PRESSURES AND CELL MASSES WERE IN BETTER AGREEMENT. BOTH THE HAND AND CONTAIN ANALYSES GAVE A FLOW-DECAY PERIOD OF ABOUT 8 S.
(2) CASES CF02 AND CF04 (LARGER HEAT SINKS THAN CF02) USED A SMALLER FLOW AREA TO GIVE A LONGER FLOW-DECAY PERIOD AND HEAT SINKS TO APPROXIMATE ISOTHERMAL CONDITIONS. IN BOTH CASES THE FLOW MATCHED HAND CALCULATIONS TO WITHIN 0.5% OVER MOST OF THE FLOW RANGE. WHEN THE FLOW DECREASED TO ABOUT 10% OF THE MAXIMUM, THE DEVIATION INCREASED TO ABOUT 40%. CASE CF02 DEVIATED FROM ISOTHERMAL BY ~0.8 K, WHILE CF04 DEVIATED BY ONLY ~0.1 K. THE CF04 RESULTS MORE CLOSELY MATCHED THE HAND CALCULATIONS OVER A GREATER PORTION OF THE FLOW RANGE THAN DID THE CF02 RESULTS. THE CELL PRESSURES AND MASSES AS A FUNCTION OF TIME FOR BOTH CF02 AND CF04 CLOSELY MATCHED THE HAND CALCULATION RESULTS OVER THE WHOLE RANGE OF THE PROBLEM. THE FLOW-DECAY PERIOD FOR BOTH CASES WAS IN GOOD AGREEMENT WITH THAT DERIVED FROM THE HAND CALCULATIONS.

FIGURES CF-01 AND CF-02 SHOW THE TEMPERATURE AND PRESSURE RESPONSES OF THE SYSTEM AS PREDICTED BY THE CONTAIN CODE. THESE RESULTS APPLY TO CASE CF04, WHICH HAD THE LARGEST HEAT SINK TO MAINTAIN THE GAS AT ESSENTIALLY ISOTHERMAL CONDITIONS.

9. COMMENTS: THE HAND ANALYSIS ASSUMED ISOTHERMAL CONDITIONS IN ORDER TO SIMPLIFY THE ANALYTICAL SOLUTION. THE CONTAIN ANALYSIS COULD NOT PRECISELY SIMULATE THE ISOTHERMAL CONDITIONS. THIS ACCOUNTS FOR SOME OF THE QUANTITATIVE DIFFERENCES BETWEEN THE CONTAIN AND HAND ANALYSES. OVERALL, THE NEAR-ISOTHERMAL CONTAIN CASES (CF02 AND CF04) GAVE RESULTS VERY CLOSE TO THOSE OF THE HAND ANALYSES. THE QUASI-STEADY-STATE-FLOW ROUTINE IN CONTAIN, THEREFORE, APPEARS TO BE WORKING PROPERLY AND GIVING GOOD RESULTS.

10. SUGGESTIONS FOR ADDITIONAL TESTS: USE DIFFERENT TIME STEPS TO DETERMINE THE EFFECT, IF ANY, ON THE RESULTS TO ANY GIVEN POINT IN TIME.

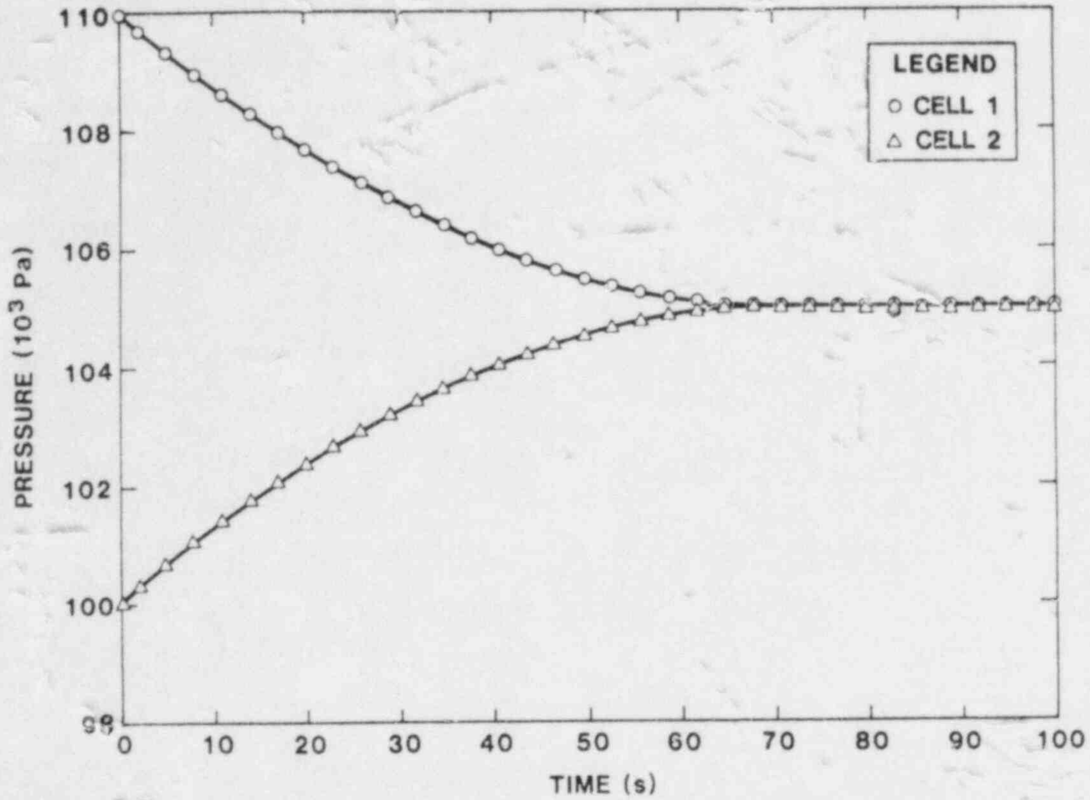

Figure CF-01 Cell pressures during isothermal intercell flow using quasi-steady flow routine (Test CF04).

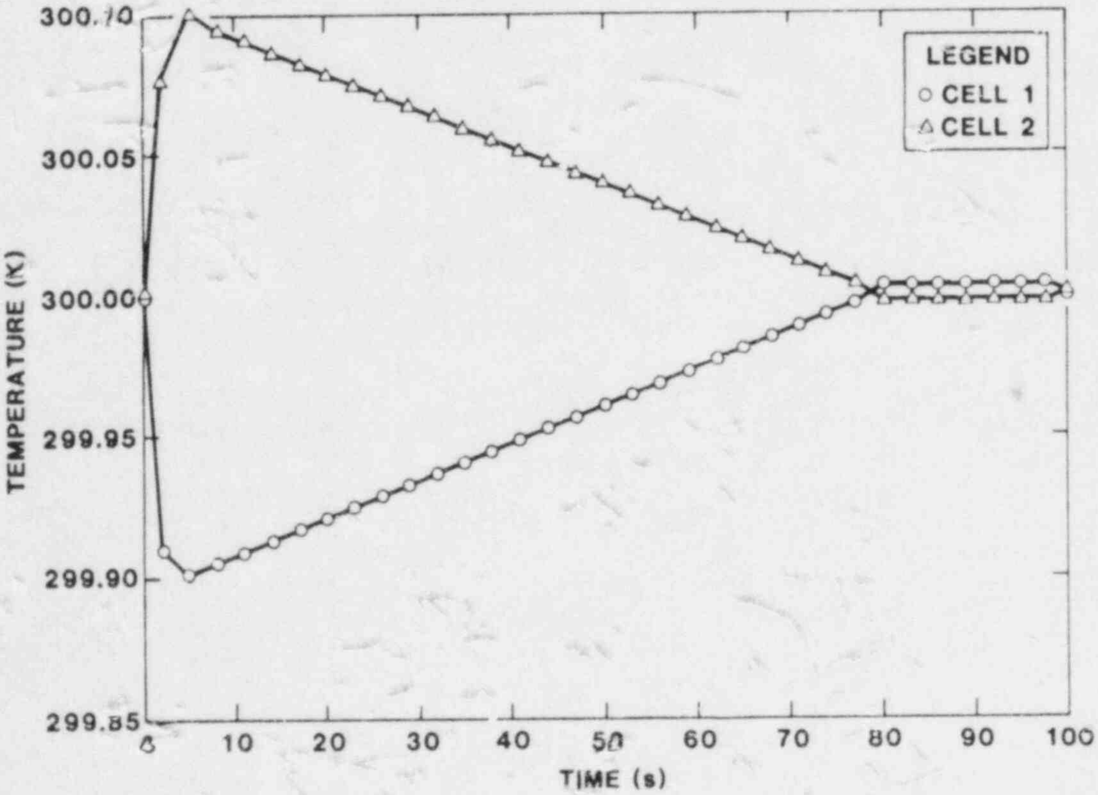

Figure CF-02 Cell gas temperatures during isothermal intercell flow using quasi-steady flow routine (Test CF04).

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: CF05(ST) USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A

3. TITLE OF TEST: INTERCELL FLOW - DEFAULT FLOW ROUTINE (INERTIAL FLOW ROUTINE)

4. CODE VERSION (DATE): DEFAULT(312) (3-23-82)

5. ACTIVE MODULES OR OPTIONS: DEFAULT FLOW ROUTINE, ATMOSPHERE THERMODYNAMICS

6. CONTAINMENT CONFIGURATION AND SOURCES: TWO EQUAL VOLUME CELLS, CELL #1 WITH AN INITIAL PRESSURE OF 1.1E5 PA, AND CELL #2 WITH AN INITIAL PRESSURE OF 1.0E5 PA. EACH CELL IS INITIALLY AT 300 K. LARGE HEAT SINKS ARE IN EACH CELL TO MAINTAIN THE GAS AS NEARLY ISOTHERMAL AS POSSIBLE. A FLOW AREA OF 0.005 SQ METERS WAS USED. THE CELLS ARE FILLED WITH HYDROGEN GAS.

7. TEST: COMPARE, AS A FUNCTION OF TIME, THE INTERCELL FLOW RATE, THE CELL PRESSURES, AND THE CELL MASSES CALCULATED BY CONTAIN WITH THOSE DERIVED FROM A SEPARATE HAND ANALYSIS. ALSO COMPARE EARLY-TIME TRANSIENT-FLOW BEHAVIOR AND LATE-TIME, LOW-PRESSURE OSCILLATORY BEHAVIOR WITH PREDICTIONS FROM SIMPLIFIED HAND ANALYSIS.

8. RESULTS OF TEST: (1) INITIAL TRANSIENT FLOW: THE SIMPLIFIED HAND CALCULATIONS PREDICTED THAT THE FLOW WOULD REACH A MAXIMUM VALUE 0.02 TO 0.5 S AFTER FLOW INITIATION. THE CONTAIN RESULTS GAVE A MAXIMUM BETWEEN 0.018 AND 0.022 S. THUS TREATMENT OF THE INITIAL TRANSIENT-FLOW BEHAVIOR IN CONTAIN IS QUITE REASONABLE.
(2) LOW-PRESSURE OSCILLATORY FLOW: THE SIMPLIFIED HAND ANALYSIS PREDICTED FLOW OSCILLATIONS WITH A PERIOD OF ABOUT 2.50 S. THE CONTAIN RESULTS SHOWED AN OSCILLATION PERIOD OF ABOUT 2.15 S. THE FLOW RATES DURING THIS PERIOD ARE VERY SMALL, SO THE NET EFFECT IS TRIVIAL. NEVERTHELESS, THE OSCILLATION PERIOD INDICATED BY THE CONTAIN RESULTS AGREES FAIRLY WELL WITH THAT FROM THE HAND ANALYSIS.
(3) OVERALL FLOW: THE PEAK FLOW RATE PREDICTED BY CONTAIN WAS 0.10255 KG/S. THE HAND ANALYSIS (WHICH IGNORED INERTIAL EFFECTS) GAVE A PEAK FLOW OF 0.10258. FOR MOST OF THE BLOWDOWN PERIOD, THE FLOW RATE PREDICTED BY CONTAIN WITH THE DEFAULT FLOW ROUTINE TRACKED THE FLOW PREDICTED BY THE HAND ANALYSIS QUITE CLOSELY, EXCEPT THAT THE CONTAIN FLOW OSCILLATED ABOUT THE VALUES FROM THE HAND ANALYSIS WITH A PERIOD OF ABOUT 20-30 S. DEVIATIONS IN THE FLOWS WERE GENERALLY LESS THAN ABOUT 5% OVER MOST OF THE FLOW RANGE. THE TIME AT WHICH THE FLOW DECAYED TO ~0 WAS 78.1 S FOR THE HAND ANALYSIS AND 81.6 S FOR THE CONTAIN ANALYSIS.
(4) OTHER PARAMETERS: THE PRESSURE AND MASS IN EACH CELL AS A FUNCTION OF TIME AS PREDICTED BY CONTAIN CLOSELY MATCHED THE VALUES GENERATED BY THE HAND ANALYSIS. DEVIATIONS OVER MOST OF THE FLOW PERIOD WERE GENERALLY ON THE ORDER OF 0.05% OR LESS.

FIGURE CF-03 PRESENTS A GRAPHICAL COMPARISON OF FLOW RATE VS TIME. THE THREE PLOTS GIVE THE RESULTS DERIVED FROM THE ISOTHERMAL ANALYTICAL SOLUTION, THE QUASI-STEADY FLOW MODEL IN CONTAIN, AND THE DEFAULT FLOW MODEL IN CONTAIN, WHICH INCLUDES THE INERTIAL FLOW TERM. THE PLOT SHOWS THAT THE THREE FLOW PREDICTIONS ARE IN FAIRLY GOOD AGREEMENT. THE PLOT ALSO ILLUSTRATES THE OSCILLATORY NATURE OF THE FLOW FROM THE DEFAULT FLOW ROUTINE IN CONTAIN RELATIVE TO THE HAND ANALYSIS RESULTS.

FIGURES CF-04 AND CF-05 SHOW THE CELL PRESSURE AND TEMPERATURE IN RESPONSE TO THE TRANSIENT FLOW.

9. COMMENTS: OVERALL, THE DEFAULT FLOW ROUTINE IN CONTAIN GAVE RESULTS THAT WERE IN REASONABLE AGREEMENT WITH HAND ANALYSES. ALTHOUGH THE FLOW RATES FROM CONTAIN EXHIBITED AN OSCILLATORY BEHAVIOR ABOUT THE FLOW RATES PREDICTED BY THE HAND ANALYSIS, VALUES FOR THE CUMULATIVE MASS TRANSFERRED UP TO ANY SPECIFIC TIME WERE IN GOOD AGREEMENT.

   WHEN USING THE DEFAULT FLOW ROUTINE IN CONTAIN, CARE MUST BE TAKEN TO USE PROBLEM TIME STEPS THAT ARE SMALLER THAN THE INITIAL TRANSIENT-FLOW TIME (A CHARACTERISTIC TIME) AND THAT ARE SMALLER THAN THE PERIOD OF THE OSCILLATIONS ASSOCIATED WITH LOW-PRESSURE CONDITIONS. (THESE TIMES CAN BE DETERMINED FROM THE CHARACTERISTICS OF THE FLOW SYSTEM BEING MODELED.) OTHERWISE, CONTAIN HAS DIFFICULTY IN REDUCING THE TIME STEP TO VALUES SUITABLE FOR THE CALCULATION. LARGE CPU TIMES ARE REQUIRED IN SUCH CASES, AND CONVERGENCE MAY NOT BE ACHIEVED AT ALL. FOR SIMILAR TEST PROBLEMS (CF04 VS CF05), THE DEFAULT FLOW ROUTINE REQUIRED FIVE TIMES AS MUCH CPU TIME AS THE QUASI-STEADY-STATE FLOW ROUTINE.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

==

1. PROBLEM: ID NO. CF05 2. LEVEL: PL01 OR PL04 3. RESOLVED? NO
4. DESCRIPTION: IF TIME STEPS ARE TOO LARGE, EITHER EXCESSIVE CPU TIMES WILL BE REQUIRED OR THE PROBLEM WILL NOT RUN AT ALL.
5. DATE PROBLEM RESOLVED:

==

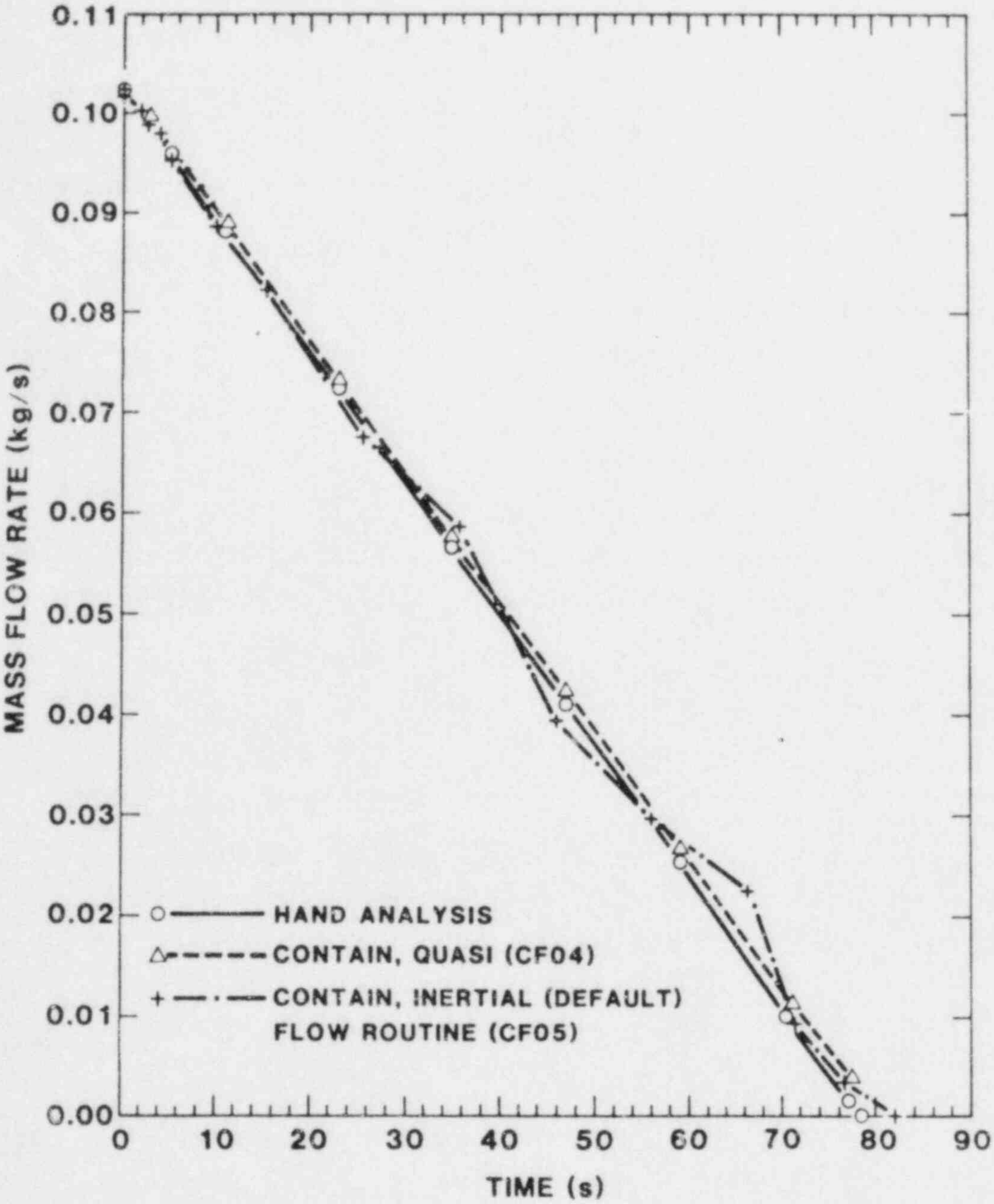

Figure CF-03 Comparison of CONTAIN'S intercell flow rates with results of hand calculations.

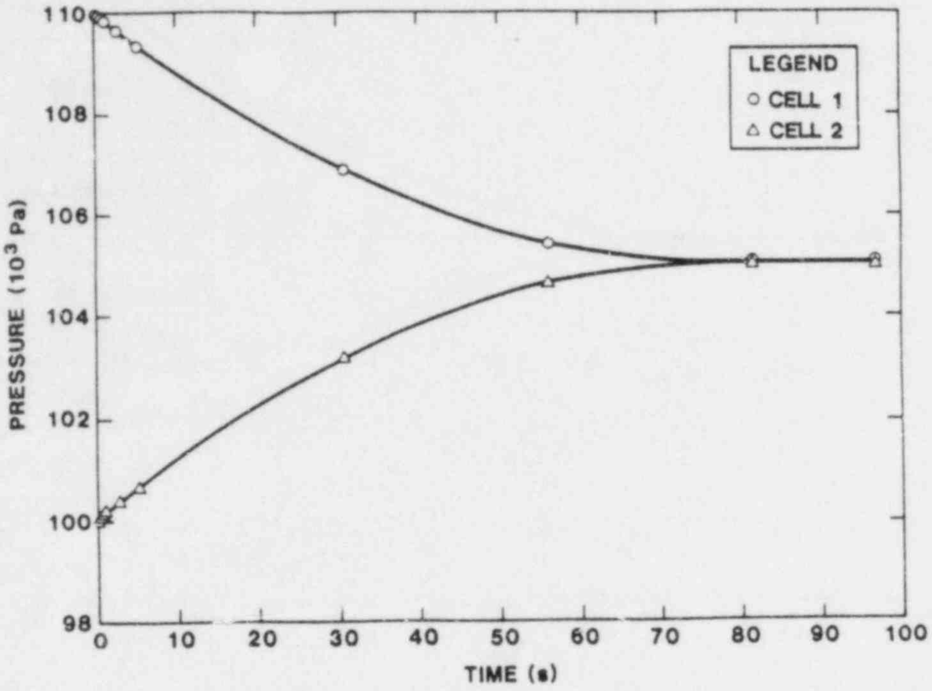

Figure CF-04 Cell pressures during isothermal intercell flow using inertial flow routine (Test CF05).

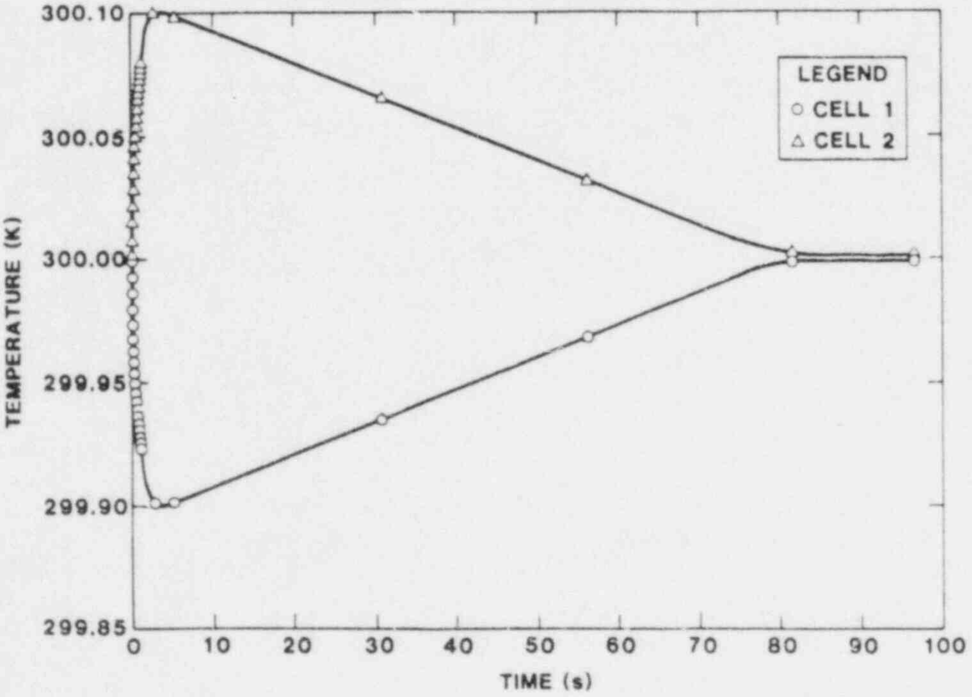

Figure CF-05 Cell gas temperatures during isothermal intercell flow using inertial flow routine (Test CF05).

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: CF06, CF07(ST) USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A

3. TITLE OF TEST: ADIABATIC INTERCELL FLOW

4. CODE VERSION (DATE): 324 (7-19-82)

5. ACTIVE MODULES OR OPTIONS: FLOW, ATMOSPHERE THERMODYNAMICS

6. CONTAINMENT CONFIGURATION AND SOURCES: TWO INTERCONNECTED CELLS WITH NO HEAT SINKS OR SOURCES (ADIABATIC). THE INITIAL CONDITIONS WERE AS FOLLOWS:

CELL #	VOLUME, CU M	TEMP, K	PRESS, PA
1	1000.0	300.0	1.500E5
2	500.0	400.0	1.000E5

THE INTERCELL FLOW AREA WAS 0.005 SQUARE METERS.

TEST CF06 UTILIZED THE DEFAULT (INERTIAL) FLOW ROUTINE IN CONTAIN. A LOSS COEFFICIENT OF 0.20 WAS USED. TEST CF07 USED THE QUASI-STEADY FLOW ROUTINE WITH A LOSS COEFFICIENT OF 0.02.

7. TEST: COMPARE THE FINAL CELL TEMPERATURES AND PRESSURES FROM CONTAIN WITH PREDICTIONS FROM HAND CALCULATIONS. THE HAND ANALYSIS ASSUMED THAT BACKFLOW DID NOT OCCUR.

8. RESULTS OF TEST: CONTAIN RESULTS CLOSELY MATCHED THE HAND ANALYSIS PREDICTIONS. THE PREDICTED END-STATE CONDITIONS FOR THE TWO CELLS AFTER PRESSURE EQUILIZATION WERE AS FOLLOWS:

	CONTAIN		HAND ANALYSIS	
	TEMP, K	PRESS, PA	TEMP, K	PRESS, PA
TEST CF06 - DEFAULT FLOW ROUTINE				
CELL #1	290.0	1.334E5	290.1	1.333E5
CELL #2	403.9	1.334E5	403.2	1.333E5
TEST CF07 - QUASI-STEADY FLOW				
CELL #1	290.2	1.333E5	290.1	1.333E5
CELL #2	403.3	1.333E5	403.2	1.333E5

FIGURE CF-06 SHOWS THE TEMPERATURE RESPONSE OF THE CELL ATMOSPHERES FOR TEST CF06. THE CORRESPONDING PRESSURE TRACE IS SHOWN IN FIGURE CF-07. FIGURES CF-08 AND CF-09 SHOW THE SAME INFORMATION FOR TEST CF07. THE PRESSURE EQUILIBRATION TIME IS SIGNIFICANTLY SHORTER FOR THE LATTER TEST BECAUSE A LOWER VALUE FOR THE LOSS COEFFICIENT IS USED.

9. COMMENTS: BOTH TESTS INDICATE THAT CONTAIN RESULTS AGREE VERY CLOSELY WITH RESULTS OF THE HAND ANALYSES FOR THE ADIABATIC FLOW PROBLEMS. USE OF THE DEFAULT FLOW ROUTINE IN CF06 PRODUCES CHARACTERISTIC OSCILLATORY

FLOW AFTER THE TWO CELL PRESSURES ARE FIRST EQUALIZED. WITH A LOW VALUE FOR THE LOSS COEFFICIENT, FLOW REVERSAL CAN BE SUBSTANTIAL AND WILL PRODUCE MORE MIXING OF THE GASES IN THE TWO CELLS THAN CAN BE INFERRED FROM THE SIMPLIFIED HAND ANALYSIS. TEST CF06 EMPLOYED A LOSS COEFFICIENT THAT HELD THIS REVERSE-FLOW MIXING TO A NEGLIGIBLE AMOUNT. OTHERWISE, THE FINAL CELL TEMPERATURES WOULD HAVE BEEN AFFECTED BY THE MIXING.

10. <u>SUGGESTIONS FOR ADDITIONAL TESTS:</u> CODE COMPARISONS FOR NONISOTHERMAL CONDITIONS.

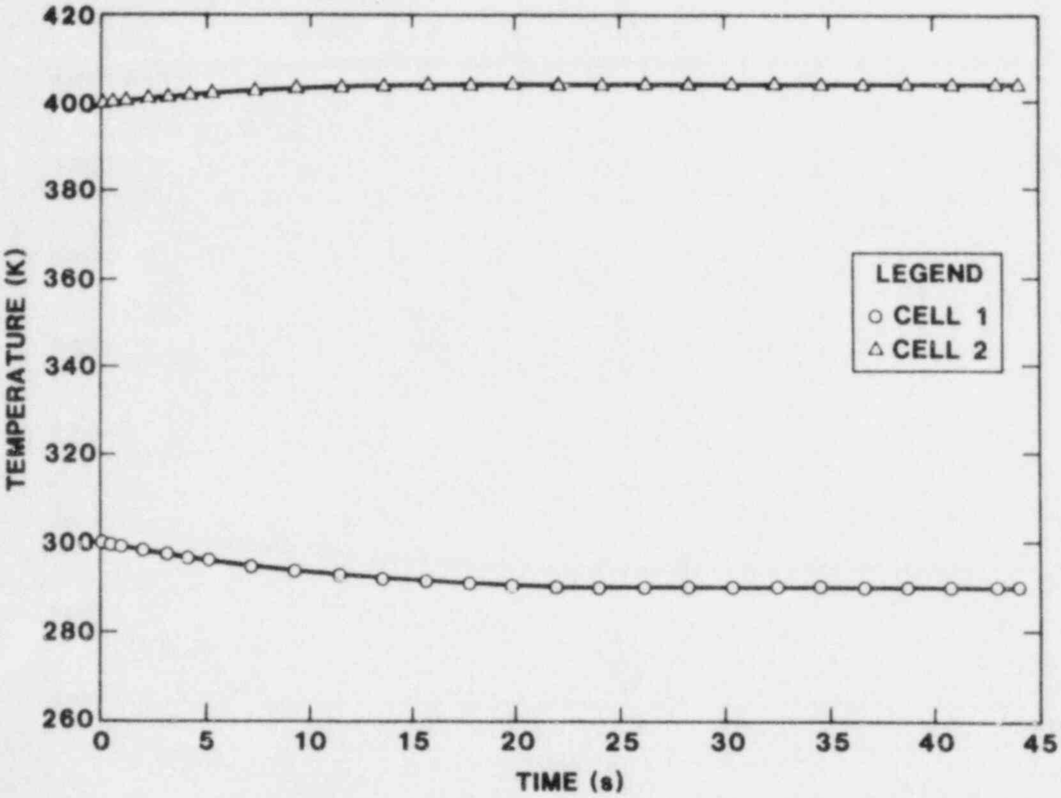

Figure CF-06 Cell gas temperatures during adiabatic intercell flow using intertial flow routine (TEST CF06, flow coefficient = 0.20).

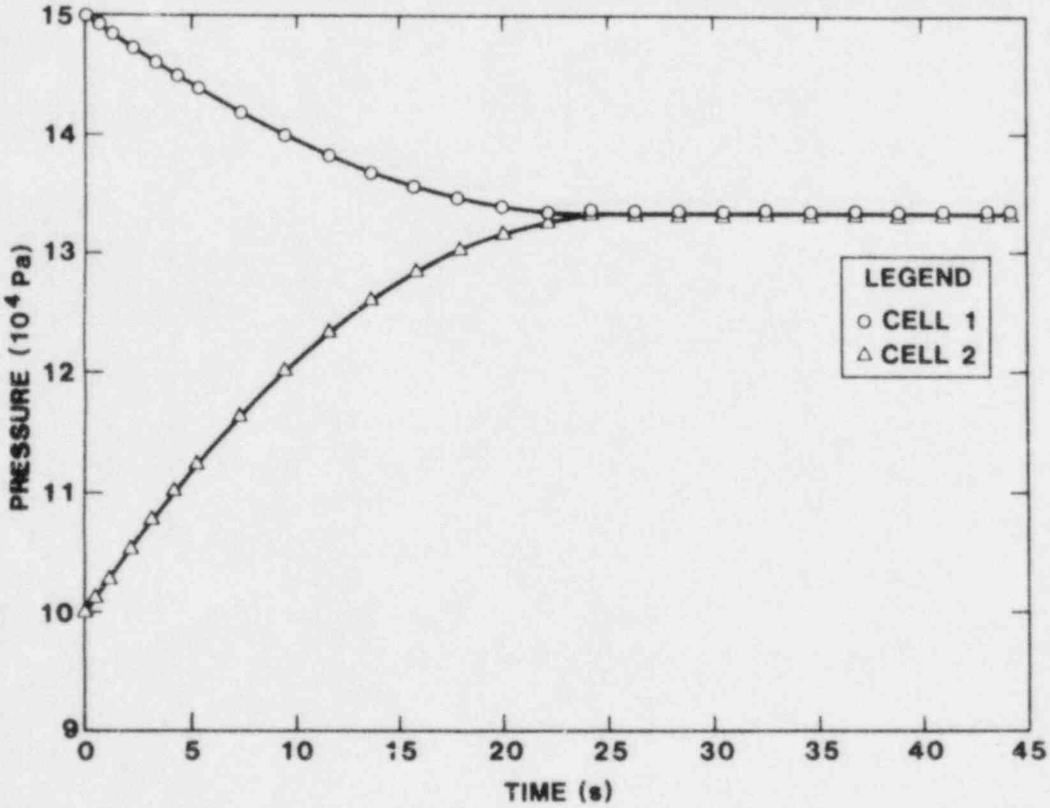

Figure CF-07 Cell pressures during adiabatic intercell flow using inertial flow routine (TEST CF06, flow coefficient = 0.20).

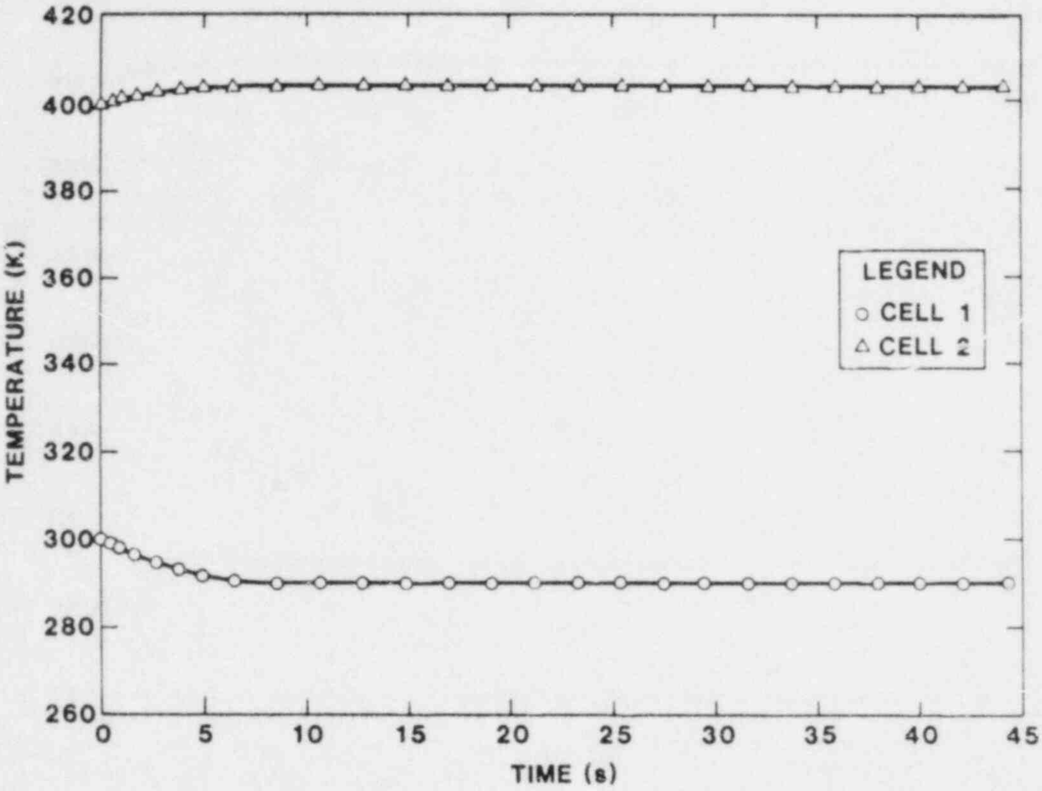

Figure CF-08 Cell gas temperatures during adiabatic intercell flow using quasi-steady flow routine (Test CF07, flow coefficient = 0.02).

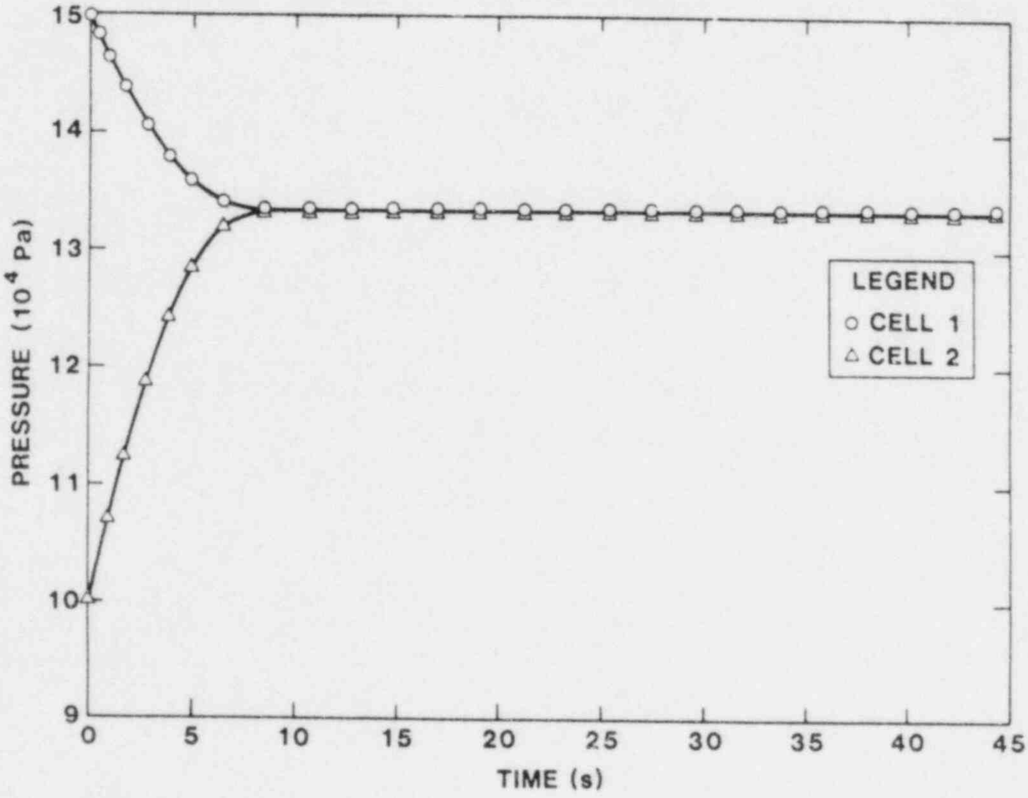

Figure CF-09 Cell pressures during adiabatic intercell flow using quasi-steady flow routine (Test CF07, flow coefficient = 0.02).

Supporting Analysis: CF Series - Intercell Flow

A. Quasi-Steady Flow Analysis - Isothermal Flow:

Consider a two-cell problem. Both cells are filled with the same gas at temperature T, but are at slightly different pressures. The two-cell system is isothermal, and there are no sources or sinks of material.

Assuming quasi-steady flow, the equations governing flow between the two cells are as follows:

$$\frac{dM_1}{dt} = - \frac{dM_2}{dt} = -W \tag{3.3-1}$$

$$P_1 - P_2 = \frac{2K|W|W}{(\rho_1 + \rho_2)A^2} \tag{3.3-2}$$

where

M_1, M_2 = mass of gas in cells 1 and 2

P_1, P_2 = pressure in cells 1 and 2

ρ_1, ρ_2 = density of gas in cells 1 and 2

A = cross-sectional area of the flow path

K = loss coefficient for the flow path

The following assumptions are also made:

1. $\rho_1 + \rho_2$ = constant
2. The flow process is isothermal
3. The gas behaves as a perfect gas, i.e., $PV = \eta RT$

The mass of gas in cell 1 as a function of time is given by:

$$M_1 = \frac{C_1(t_e - t)^2(V_1 + V_2)}{4V_1V_2} + \frac{M_TV_1}{V_1 + V_2} \text{ for } t < t_e \tag{3.3-3}$$

where

$$C_1 = \frac{RT(\rho_1 + \rho_2)A^2}{2GK}$$

$$t_e = \frac{2V_1V_2}{V_1 + V_2} \; \frac{1}{C_1^{\,0.5}} \left[\frac{M_{1o}(V_1 + V_2)}{V_1V_2} - \frac{M_T}{V_2}\right]^{1/2}$$

G = molecular weight of gas

M_{1o} = initial mass of gas in cell 1 at $t = 0$

$M_T = M_1 + M_2$

V_1, V_2 = volumes of cells 1 and 2

R = gas constant

T = system temperature (assumed constant)

t_e = the time at which the pressures in the two cells equilibrate and the flow stops.

The mass flow rate at any time, t, is given by:

$$W = -\frac{dM_1}{dt} = \frac{C_1(V_1 + V_2)}{2V_1V_2}(t_e - t) \qquad (3.3\text{-}4)$$

B. Analysis Considering Flow Inertia (Test CF05) - Isothermal Flow:

The basic relationship below describes the intercell flow:

$$\frac{L}{A}\frac{dW}{dt} = P_1 - P_2 - \frac{2K|W|W}{\left(\frac{M_1}{V_1} + \frac{M_2}{V_2}\right)A^2} \qquad (3.3\text{-}5)$$

where

L = inertial length of the flow path.

If the flow path connecting the two cells is opened very suddenly, the initial pressure differential is assumed to remain approximately constant for the initial transient period, i.e., $(P_1 - P_2)_o \sim$ const.

For this period,

$$\frac{dW}{dt} = \frac{A}{L}(P_1 - P_2)_o - \frac{2K|W|W}{\left(\frac{M_1}{V_1} + \frac{M_2}{V_2}\right)AL} \qquad (3.3\text{-}6)$$

With the initial condition $W = 0$ at $t = 0$, the initial flow rate is given by the expression

$$W = W_o \tanh(t/t_T) \qquad (3.3\text{-}7)$$

where

$$W_o = 2\, M_o/t_e$$

$$M_o = \frac{V_1 V_2}{V_1 + V_2} \; \frac{G(P_1 - P_2)_o}{RT}$$

$$t_T = L\left[\frac{G(P_1 - P_2)_o}{2KRT\ (P_1 + P_2)_o}\right]^{1/2}$$

t_e is as previously defined, and t_T is the rise time of the flow as the flow path is suddenly opened.

After the initial transient, the flow steadily decays until the pressure differential becomes very small. During this quasi-steady period the flow rate can be represented by the expression:

$$W = W_o(1 - \frac{t}{t_e}) \quad \text{for } t < t_e \tag{3.3-8}$$

When the pressure difference between the two cells becomes very small, the flow velocity will become very small. For this situation the flow can be approximated as follows:

$$\frac{d^2M}{dt^2} + \frac{RTA\ (V_1 + V_2)}{GL(V_1 V_2)}\, M = 0 \tag{3.3-9}$$

The solutions of this equation are sine waves with a frequency

$$\omega = 2\pi/t_I = \left[\frac{RTA\ (V_1 + V_2)}{GL(V_1 V_2)}\right]^{1/2} \tag{3.3-10}$$

For the time $t > t_e$, the flow should oscillate with an oscillation period t_I.

C. Adiabatic Flow Test:

For the case of abiabatic intercell flow of an ideal gas, the end-state conditions are given by the following relationships:

Final pressure:

$$P_f = \frac{P_{1_o} V_1 + P_{2_o} V_2}{V_1 + V_2} \tag{3.3-11}$$

Final temperature in cell 1:

$$T_{1_f} = \left(\frac{P_{1_o}(V_1 + V_2)}{P_{1_o}V_1 + P_{2_o}V_2}\right)^{\left(\frac{1-\gamma}{\gamma}\right)} T_{1_o} \qquad (3.3\text{-}12)$$

Final temperature in cell 2:

$$T_{2_f} = \frac{P_f V_2}{\frac{P_{1_o} V_1}{T_{1_o}} + \frac{P_{2_o} V_2}{T_{2_o}} - \frac{P_f V_1}{T_{1_f}}} \qquad (3.3\text{-}13)$$

where

P_{1_o} = initial pressure in cell 1

T_{1_o} = initial temperature in cell 1

P_{2_o} = initial pressure in cell 2

T_{2_o} = initial temperature in cell 2

V_1, V_2 = cell volumes

γ = gas specific heat ratio: C_p/C_v

```
&&       ------------------ CF04(ST) -----------------------------------------------
 CONTROL=9 2 3 1 4 2 20 0 0 0
 MATERIAL
 COMPOUND N2 O2 H2 HE NAV NAL   FE
 FISSION
 TE132 I132
 I133 XE133
 TIMES 50.0 0.0 1.0 2.0 100.0 1.0 1.0
 FLOWS
   AREA(1,2)=0.005 AVL(1,2)=0.05  CFC(1,2)=2.0  TOPEN(1,2)=0.0  QUASI
 PRFISS PRFLOW
 FISSION 0 0  2 2
 TE132 I132
 I133 XE133
 1.0E5 2.0E5
 1.0E5 1.0E6
 1.0 1.0 1.0 1.0
 FPM-CELL=1
 HOST=GAS 1.0 1.0 1.0 1.0
 EOI
 TITLE
        INTERCELL GAS FLOW TESTS
        CASE CF04:  QUASI-STEADY FLOW BETWEEN EQUAL VOLUME CELLS
      SIMILAR TO CF02 BUT LARGER HEAT SINKS ADDED TO KEEP CLOSER TO 300 K
 FAST
 CELL=1
 CONTROL=18 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 TITLE
    HIGH PRESSURE CELL (#1)
 GEOMETRY
 1000.0 10.0
 ATMOS=1
 1.1E5 300.0
 H2 1.0
 &&   ----------- LARGE HEAT SINK --------------------------------
 STRUC
    HEATSINK
    WALL
    SLAB 3 1 300.0 1.0 0 1.0E5
    0.0 0.005 0.010 0.015
    FE FE FE
 CELL = 2
 CONTROL=18 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 TITLE
    LOW PRESSURE CELL (#2)
 GEOMETRY
 1000.0 10.0
 ATMOS=1
 1.0E5 300.0
 H2 1.0
```

```
-------------CELL #2 HEAT SINK ------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 2 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
   FE FE FE
EOF
```

```
&&      ------------------ CF05(ST) ----------------------------------
CONTROL=9 2 3 3 4 2 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL   FE
FISSION
TE132 I132
I133 XE133
TIMES 250.0 0.0 C.001 0.01 1.0 0.01 0.5 5.0 0.1 5.0 100.0 1.0 1.0
FLOWS
  AREA(1,2)=0.005 AVL(1,2)=0.0025  CFC(1,2)=2.0  TOPEN(1,2)=0.0
PRFISS PRFLOW
FISSION 0 0  2 2
TE132 I132
I133 XE133
1.0E5 2.0E5
1.0E5 1.0E6
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 1.0 1.0
EOI
TITLE
       INTERCELL GAS FLOW TESTS
       CASE CF05:  NEAR ISOTHERMAL FLOW BETWEEN EQUAL VOLUME CELLS
   SAME AS CF04 EXCEPT USES REFERENCE FLOW ROUTINE RATHER THAN QSS
FAST
CELL=1
CONTROL=18 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
   HIGH PRESSURE CELL (#1)
GEOMETRY
1000.0 10.0
ATMOS=1
1.1E5 300.0
H2 1.0
&&      ----------- LARGE HEAT SINK --------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 1 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
   FE FE FE
CELL = 2
CONTROL=18 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
   LOW PRESSURE CELL (#2)
```

```
GEOMETRY
1000.0 10.0
ATMOS=1
1.0E5 300.0
H2 1.0
&&      -------------CELL #2 HEAT SINK --------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 2 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
   FE FE FE
EOF
```

```
&&      ------------------ CF07(ST) -------------------------------------
CONTROL=9 2 3 3 4 2 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL   FE
FISSION
TE132 I132
I133 XE133
TIMES 55.00 0.0 0.0500 0.20 1.0 0.050 0.5 5.0 0.050 1.0 45.00 1.0 1.0
FLOWS
  AREA(1,2)=0.005 AVL(1,2)=0.0025  CFC(1,2)=0.02  TOPEN(1,2)=0.0 QUASI
PRFISS PRFLOW
FISSION 0 0  2 2
TE132 I132
I133 XE133
1.0E5 2.0E5
1.0E5 1.0E6
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 1.0 1.0
EOI
TITLE
       INTERCELL GAS FLOW TESTS    --  ADIABATIC CASE
CASE CF07(ST): ADIABATIC FLOW; CELL #1 = 1000 , CELL #2 VOL = 500
  FRICTION COEF OF 0.02
FAST
CELL=1
CONTROL=18 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
   HIGH PRESSURE CELL (#1)
GEOMETRY
1000.0 10.0
ATMOS=1
1.5E5 300.0
H2 1.0
&&      ----------- LARGE HEAT SINK --------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 1 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
```

```
   FE FE FE
HT-TRAN OFF OFF OFF OFF OFF OFF OFF
CELL = 2
CONTRO=18 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
   LOW PRESSURE CELL (#2)
GEOMETRY
500.00 10.0
ATMOS=1
1.0E5 400.0
H2 1.0
&&      -------------CELL #2 HEAT SINK --------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 2 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
   FE FE FE
HT-TRAN OFF OFF OFF OFF OFF OFF OFF
EOF
```

3.3.2 Series AF - Intercell Flow of Aerosols

The tests in this series exercised CONTAIN's handling of aerosol transport from one cell to another via gas flow between two cells. These tests were intended to check only this intercell movement of aerosols, not the overall behavior of aerosols. The AF series of tests employed the same flow arrangement and conditions as were used in the CF series tests. Here, however, aerosols were added to the atmosphere in the high pressure cell. The quasi-steady flow model was used. In addition, isothermal conditions were simulated. The hand analysis used to check the CONTAIN results ignored aerosol deposition. The test results indicate that CONTAIN is handling intercell transport of aerosols correctly, at least for a two-cell system. Systems of more than two cells have not yet been included in this test series.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: AF01, AF02, AF03, & AF04(ST) USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: AEROSOL FLOW (INTERCELL TRANSPORT OF AEROSOLS)
4. CODE VERSION (DATE): 324 (4-9,29,30-82)
5. ACTIVE MODULES OR OPTIONS: INTERCELL FLOW, ATMOSPHERE THERMODYNAMICS, AND AEROSOL BEHAVIOR (MAEROS)
6. CONTAINMENT CONFIGURATION AND SOURCES: TWO EQUAL VOLUME CELLS, CELL #1 WITH AN INITIAL PRESSURE OF 1.1E5 PA AND CELL #2 WITH AN INITIAL PRESSURE OF 1.0E5 PA. EACH CELL IS INITIALLY AT 300 K. THERE ARE LARGE HEAT SINKS IN BOTH CELLS TO MAINTAIN ESSENTIALLY ISOTHERMAL CONDITIONS (FOR BETTER COMPARISON WITH SIMPLIFIED HAND ANALYSIS OF FLOW AND AEROSOL TRANSPORT). CELL #1 CONTAINS AN AEROSOL AT AN INITIAL CONCENTRATION OF 1 GM/M**3.
7. TEST: DETERMINE AS A FUNCTION OF TIME THE TOTAL MASS OF AEROSOL TRANSPORTED FROM CELL #1 TO CELL #2 WITH THE GAS FLOW. COMPARE THE CONTAIN RESULTS WITH THOSE DERIVED FROM HAND ANALYSIS. THE SPECIFIC CHARACTERISTICS OF THE DIFFERENT CASES RUN ARE AS FOLLOWS:

TEST #	GAS	FLOW AREA, M**2	AEROSOL MEAN DIAMETER, M
AF01	H2	0.005	0.5E-6
AF02	N2	0.02	0.5E-6
AF03	N2	0.02	0.1E-6
AF04	N2	0.02	2.0E-6

THE DIFFERENT TESTS WERE RUN TO FIND CONDITIONS THAT WOULD MINIMIZE AEROSOL DEPOSITION AS CALCULATED BY CONTAIN. THE HAND CALCULATIONS ASSUMED THAT DEPOSITION OF AEROSOLS DID NOT OCCUR.

8. RESULTS OF TEST: BECAUSE THE HAND CALCULATIONS DID NOT TAKE AEROSOL DEPOSITION INTO ACCOUNT, THE COMPARISON WITH THE CONTAIN RESULTS WAS USEFUL ONLY WHEN DEPOSITION EFFECTS WERE MINIMIZED IN THE CONTAIN ANALYSIS. CUMULATIVE AEROSOL DEPOSITION IN CELL #1 UP TO THE TIME OF PRESSURE EQUILIBRATION BETWEEN THE TWO CELLS RANGED FROM A LOW OF ABOUT 2% TO A HIGH OF ABOUT 33% FOR THE FOUR TESTS RUN. TEST AF04 EXHIBITED THE LEAST DEPOSITION (~2%), AND THUS THIS TEST WAS CHOSEN FOR COMPARISON WITH THE HAND ANALYSIS, WHICH DID NOT TAKE DEPOSITION INTO ACCOUNT. THE FOLLOWING RESULTS SHOW THE TOTAL AEROSOL MASS TRANSPORTED INTO CELL #2 AT DIFFERENT TIMES:

	TOTAL AEROSOL MASS IN CELL #2, KG	
TIME, S	CONTAIN	CALCULATED
20	0.02132	0.02147
41	0.03634	0.03669
62	0.04440	0.04397
71	0.04502	0.04542

THESE VALUES INDICATE THAT THE CONTAIN RESULTS AGREE WITH THOSE OF THE HAND ANALYSIS TO WITHIN ABOUT 1%. THE HAND ANALYSIS PREDICTED GREATER AEROSOL TRANSPORT THAN CONTAIN. THIS IS TO BE EXPECTED BECAUSE THE AEROSOL CONCENTRATION IN THE GAS AS CALCULATED BY CONTAIN WAS LESS THAN THAT ASSUMED IN THE HAND ANALYSIS BY VIRTUE OF THE DEPOSITION PROCESSES INCLUDED IN CONTAIN.

IN THIS TEST, THE CELL PRESSURES EQUILIBRATE, AND THUS THE FLOW ESSENTIALLY STOPS AT ABOUT 72 S AFTER FLOW INITIATION. FIGURE AF-01 SHOWS TOTAL AEROSOL CONCENTRATION VS TIME. AS WOULD BE EXPECTED FROM THE FLOW CONDITIONS, THE CONCENTRATION OF THE AEROSOL IN CELL #2 PEAKS AT ABOUT 70 S. THIS IS SHOWN MORE CLEARLY IN FIGURE AF-02. FIGURE AF-03 SHOWS AEROSOL DEPOSITION IN THE TWO CELLS. THE DEPOSITION IS SMALL OVER THE TIME SCALE OF THE PROBLEM. NEVERTHELESS, IT DOES CONTRIBUTE TO THE DIFFERENCES BETWEEN THE CONTAIN RESULTS AND THOSE FROM THE HAND ANALYSIS.

9. COMMENTS: THIS COMPARISON INDICATES THAT CONTAIN IS HANDLING THE INTERCELL TRANSPORT OF AEROSOLS IN A REASONABLE AND ACCURATE MANNER.

10. SUGGESTIONS FOR ADDITIONAL TESTS: TEST SYSTEMS WITH SEVERAL INTERCONNECTED CELLS, WITH BOTH PARALLEL AND SERIES INTERCONNECTIONS.

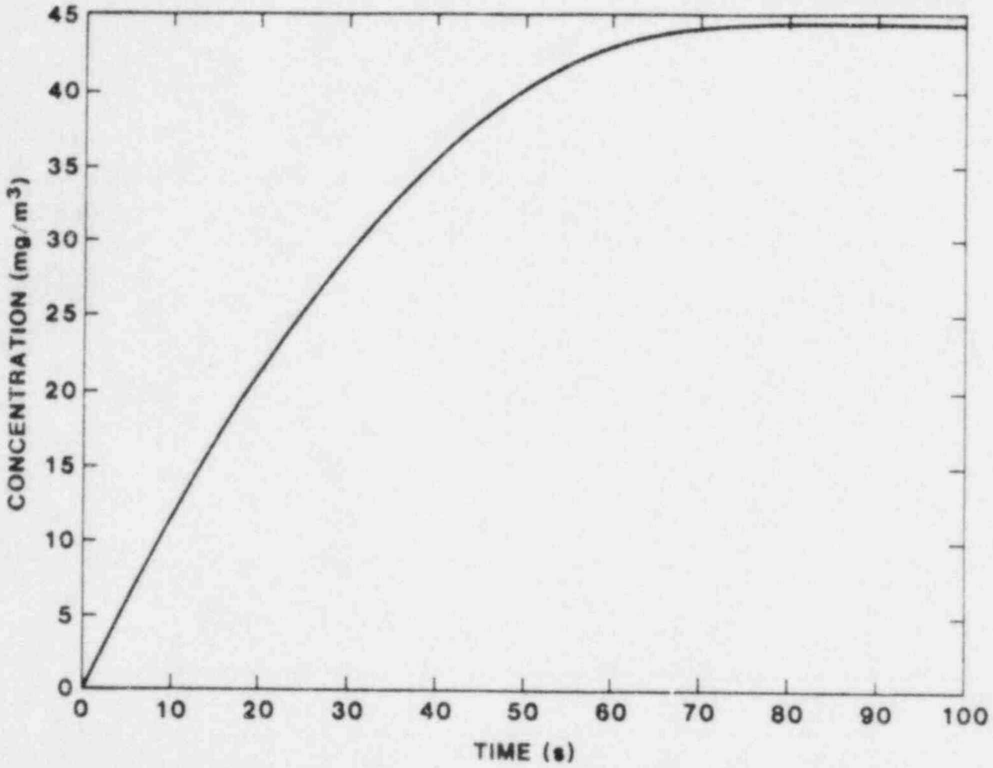

Figure AF-01 Total aerosol concentration during intercell flow of aerosols using quasi-steady flow routine (Test AF04).

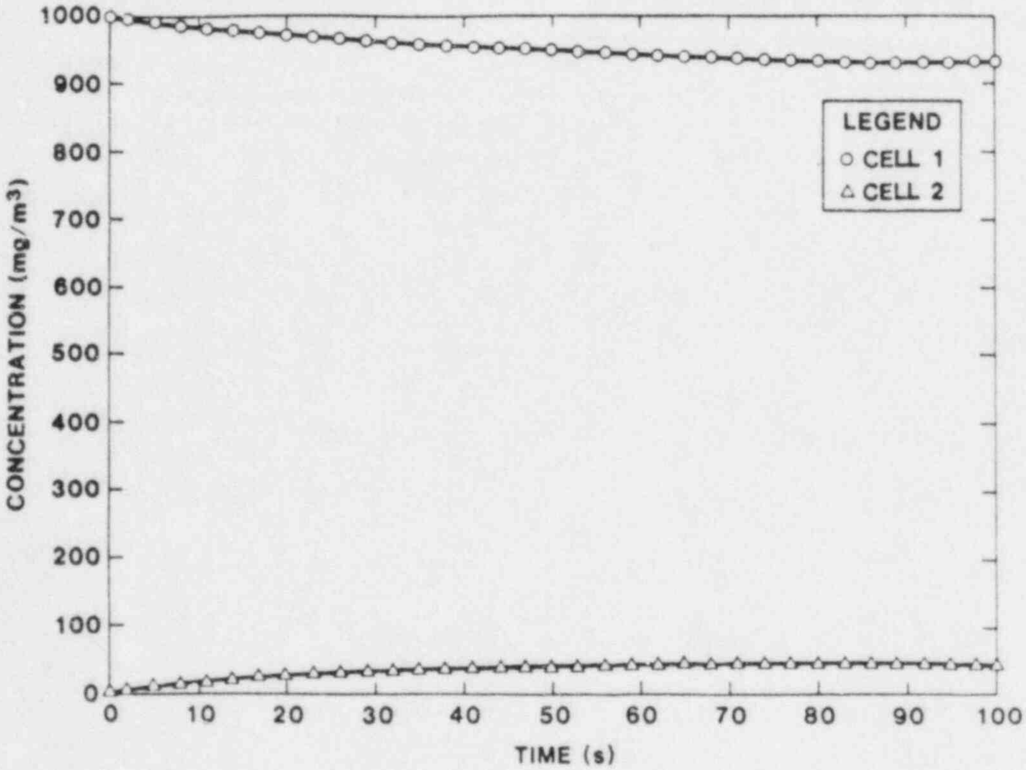

Figure AF-02 Aerosol concentration in cell 2 during intercell flow of aerosols using quasi-steady flow routine (Test AF04).

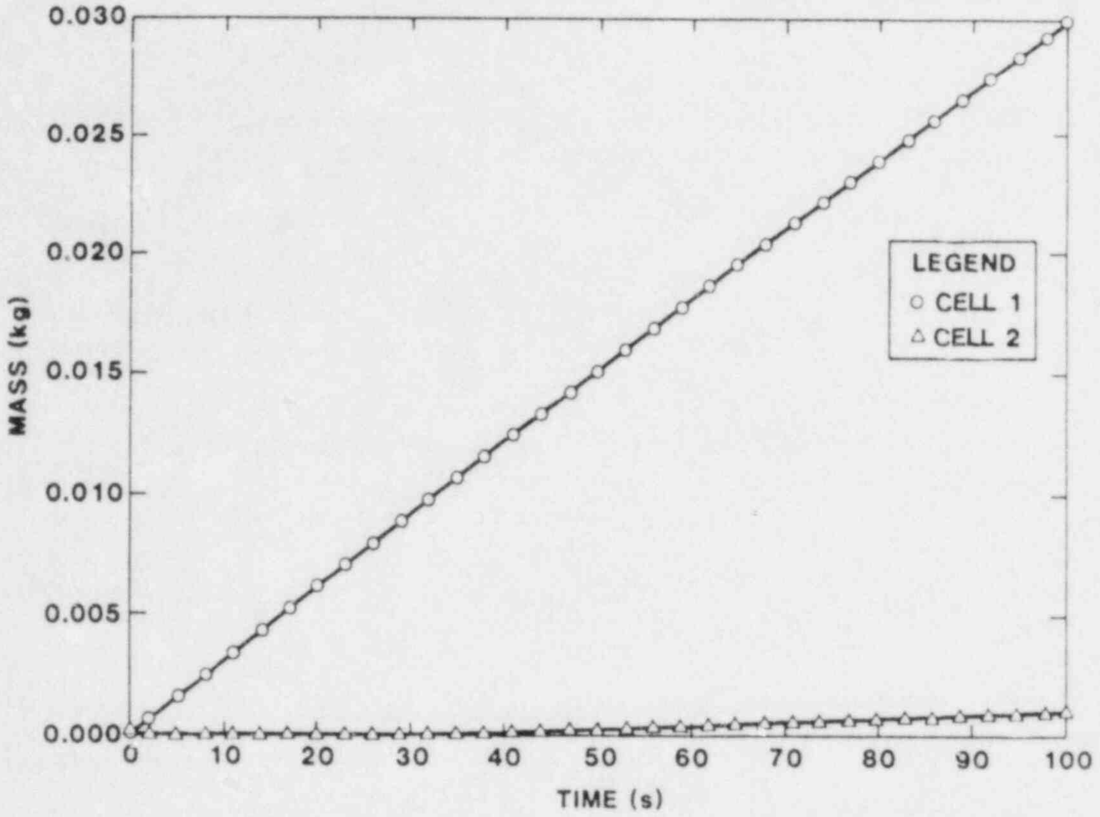

Figure AF-03 Total aerosol mass deposited during intercell flow of aerosols using quasi-steady flow routine (Test AF04).

Supporting Analysis: AF Series - Intercell Flow of Aerosols

Consider a two-cell system. Both cells are filled with the same gas at temperature T, but cell 1 is at a slightly higher pressure than cell 2. The gas in cell 1 is laden with aerosols; cell 2 is clean. The object is to predict the amount of aerosols transported from cell 1 to cell 2 as a function of time once the intercell flow path is opened.

The following simplifying assumptions are made:

1. The aerosol in cell 1 is uniformly spread throughout the cell atmosphere.
2. Aerosol deposition in cell 1 is small and can be neglected.
3. The flow is isothermal.

Using these assumptions, the mass of aerosol transported to cell 2 from cell 1 is proportional to the gas flow between the two cells, i.e.,

$$M_{A_2} = M_{A_{1_o}} \frac{\Delta M_1(t)}{M_{1_o}} \qquad (3.3\text{-}14)$$

where

$\Delta M_1(t) = M_{1_o} - M_1(t).$

The mass of gas remaining in cell 1, $M_1(t)$, is given by

$$M_1(t) = \frac{C_1(V_1 + V_2)(t_e - t)^2}{4\ V_1V_2} + \frac{M_T\ V_1}{V_1 + V_2} \quad \text{for } t < t_e \qquad (3.3\text{-}15)$$

where

$$C_1 = \frac{RT(\rho_1 + \rho_2)_o A^2}{2\ GK}$$

$$t_e = \frac{2\ V_1V_2}{(V_1 + V_2)\ C_1{}^{0.5}} \left. \frac{M_{1_o}(V_1 + V_2)}{V_1V_2} - \frac{M_T}{V_2} \right.^{1/2}$$

G = molecular weight of gas
V_1, V_2 = cell volumes
T = system temperature (assumed constant)
R = gas constant
M_{1_o} = initial mass of gas in cell 1 at $t = 0$
$M_T = M_1 + M_2$ = constant

$(\rho_1 + \rho_2)_o$ = sum of initial gas densities at $t = 0$

R = gas constant

K = loss coefficient for the flow path

A = area of flow path.

The mass of aerosol transported to cell 2 is given by

$$M_{A_2} = M_{A_{1_o}} \frac{M_{1_o} - M_1(t)}{M_{1_o}}$$

$$= \frac{M_{A_{1_o}}}{M_{1_o}} \left[M_{1_o} - \frac{C_1(t_e - t)^2(V_1 + V_2)}{4\, V_1 V_2} - \frac{M_T\, V_1}{V_1 + V_2} \right] \qquad (3.3\text{-}16)$$

where

$M_{A_{1_o}}$ = initial mass of aerosol in cell 1.

SERIES AF STANDARD TEST INPUT DATA SET

```
&&      ------------------ AF04(ST) ----------------------------------------

CONTROL=9 2 4 1 4 2 20 1 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL   FE  NA20
FISSION
TE132 I132
I133 XE133
TIMES 50.0 0.0 1.0 2.0 100.0 1.0 1.0
FLOWS
  AREA(1,2)=0.020 AVL(1,2)=0.05  CFC(1,2)=2.0  TOPEN(1,2)=0.0  QUASI
PRFISS PRFLOW  PRAER
FISSION 0 0  2 2
TE132 I132
I133 XE133
1.0E5 2.0E5
1.0E5 1.0E6
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 1.0 1.0
EOI
AEROSOL 0 0 0 0 0 0 0 NA20 =2.0E-6 0.0
TITLE
       TEST OF AEROSOL FLOW
   CASE AF04:  INITIAL CONCENTRATION OF 1000 MG/M**3 IN CELL #1
    QUASI-STEADY FLOW BETWEEN CELLS.  CELL FLOW SETUP SIMILAR TO CASE CF04.
SAME AS CASE AF02 EXCEPT LARGER AEROSOL PARTICLE SIZE FOR DEPOSITION EFFECT.
FAST
CELL=1
CONTROL=17 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
   HIGH PRESSURE CELL (#1)
GEOMETRY
1000.0 10.0
ATMOS=1
1.1E5 300.0
N2 1.0
&&      ----------- LARGE HEAT SINK ---------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 1 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
   FE FE FE
AEROSOL=1 NA20 1.0
CELL = 2
CONTROL=17 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
   LOW PRESSURE CELL (#2)
GEOMETRY
1000.0 10.0
```

```
ATMOS=1
1.0E5 300.0
N2 1.0
&&      ------------CELL #2 HEAT SINK ------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 2 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
   FE FE FE
EOF
```

3.4 FISSION-PRODUCT TESTS

3.4.1 Series FP - Fission-Product Decay and Release

The tests in this series provided both qualitative and quantitative checks on the code's treatment of fission products. Tests FP01, FP03, and FP09 employed a five-element fission-product decay chain. The first element in the chain was given a much longer half-life than the immediate daughter. These tests were performed to check (1) the basic behavior of this chain, (2) the sensitivity of the results to problem time-step size, and (3) mass conservation for the case of decay along with release from the host material.

Tests FP02 and FP04 through FP08 modeled two-element decay chains with arbitrary decay constants. The hand analyses for these tests employed an exact analytical solution for the quantity of the fission products remaining as a function of time. The release of fission products from one host material and their acceptance by another host material was also evaluated, as was the effect of problem time-step size.

The test results show that CONTAIN is handling fission-product decay, release, and acceptance quite well. Gross time-step sizes can lead to erroneous results. However, by using reasonable care in choosing appropriate time-step sizes, problems in this area can be avoided.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FP01 USER NAME: F. SCIACCA

2. TEST LEVEL: TL2, TL4A

3. TITLE OF TEST: FISSION-PRODUCT DECAY (5-ELEMENT DECAY CHAIN)

4. CODE VERSION (DATE): 208 (2/10/82)

5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO STRUCTURES.

7. TEST: SPECIFIED A SINGLE, 5-ELEMENT FISSION-PRODUCT DECAY CHAIN; ORIGINAL PARENT WAS GIVEN A MUCH LONGER HALF-LIFE THAN THE IMMEDIATE DAUGHTER. STARTED WITH ONE KG MASS OF DUM1 (FIRST ELEMENT IN DECAY CHAIN), 0 MASS FOR OTHER FISSION PRODUCTS. FOLLOWED DECAY (MASSES) OF EACH ELEMENT VS TIME TO SEE HOW RESULTS COMPARED WITH APPROXIMATE ANALYTICAL SOLUTION.

8. RESULTS OF TEST: CONTAIN AND HAND-CALCULATED VALUES FOR EARLY DECAY TIMES ARE NOT IN VERY GOOD AGREEMENT. LATER VALUES ARE IN FAIRLY CLOSE AGREEMENT. SAMPLE COMPARISONS OF THE CONTAIN VS CALCULATED RESULTS ARE AS FOLLOWS:

	REMAINING MASS			
ELEMENT	TIME = 2.0E6 S		TIME = 10.0E6 S	
NAME	CALCULATED	CONTAIN	CALCULATED	CONTAIN
DUM1	0.9570	0.9570	0.8027	0.8027
DUM2	0.00509	0.005114	0.004268	0.004291

	REMAINING MASS			
ELEMENT	TIME = 2.0E6 S		TIME = 10.0E6 S	
NAME	CALCULATED	CONTAIN	CALCULATED	CONTAIN
DUM3	0.004785	0.004825	0.004014	0.004055
DUM4	0.01914	0.01563	0.01605	0.01655
DUM5	0.0957	0.01528	0.08027	0.07481

THE CONTAIN RESULTS SHOWING THE DECAY OF THE PARENT AND THE BUILDUP AND DECAY OF THE DAUGHTER PRODUCTS ARE PRESENTED IN FIGURES FP-01 THROUGH FP-05. THE FIRST THREE DAUGHTER PRODUCTS SHOW THE CHARACTERISTIC BUILDUP AND THEN THE GRADUAL DECAY. THE LAST DAUGHTER PRODUCT HAD A RELATIVELY LONG HALF-LIFE COMPARED TO THE OTHERS. ITS PEAK MASS HAD NOT BEEN REACHED AT THE TIME THE CALCULATION WAS TERMINATED.

9. COMMENTS: CONTAIN RESULTS APPEAR TO BE VALID FOR THIS PROBLEM (AS NEAR AS CAN BE CHECKED USING APPROXIMATE ANALYTICAL SOLUTION).

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

NOTE: FIGURES FOR ALL FISSION-PRODUCT TESTS SHOW COMPUTER-GENERATED PLOTS OF THE MASS DEPOSITED IN THE POOL (LABELED "CAVITY"). BECAUSE NO POOL WAS INCLUDED IN THESE TESTS, THE PLOTS FOR THE CAVITY SHOW ZERO MASS DEPOSITED.

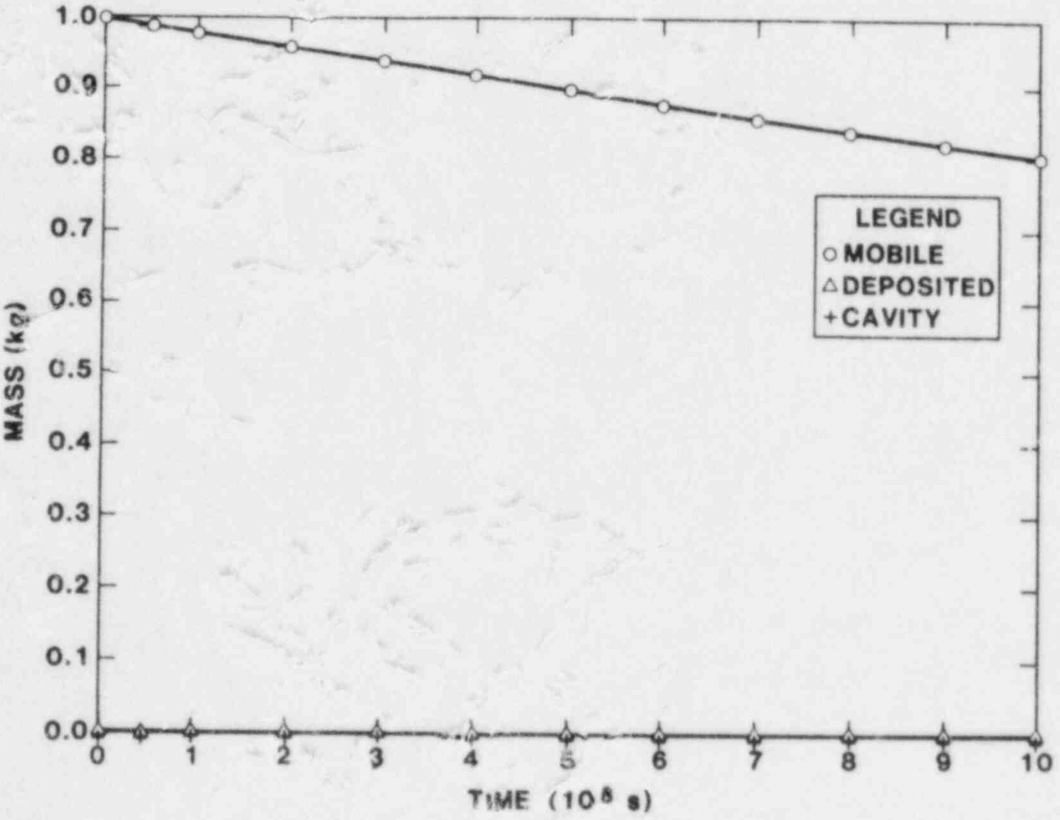

Figure FP-01 Decay of fission product DUM1 (Test FP01).

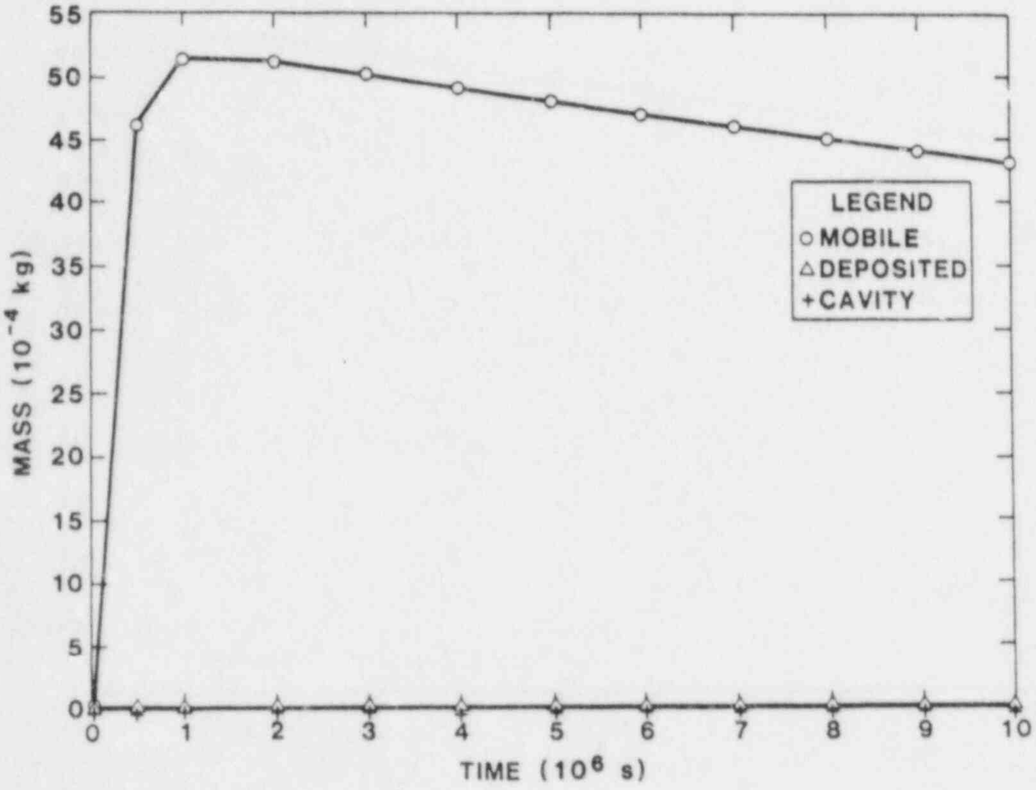

Figure FP-02 Decay of fission product DUM2 (Test FP01).

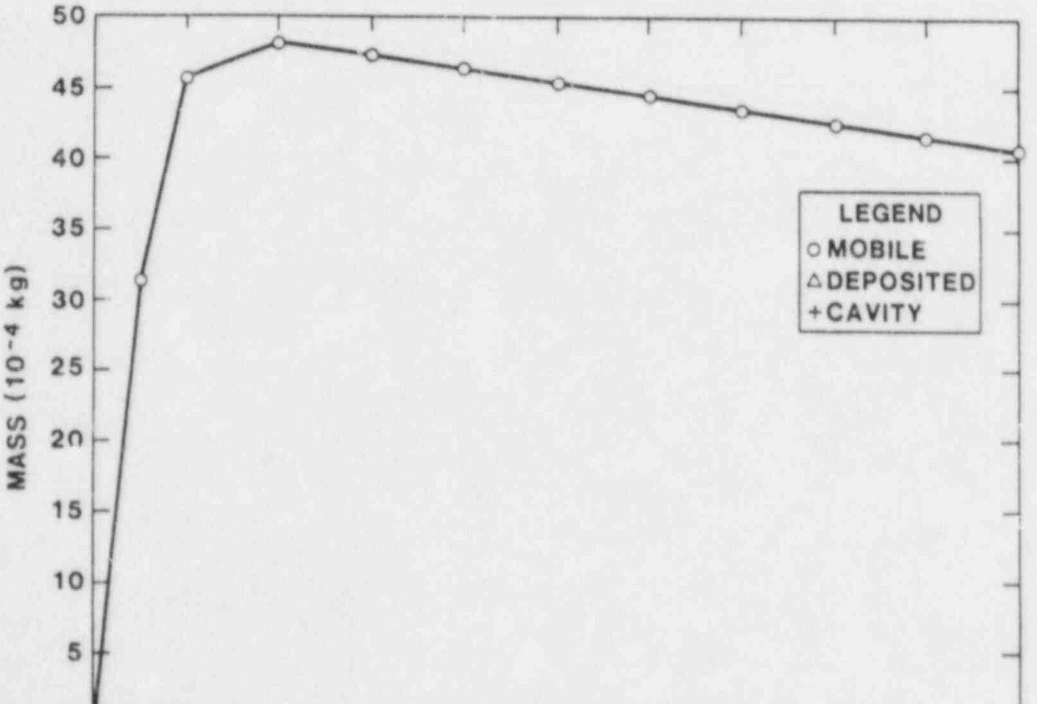

Figure FP-03 Decay of fission product DUM3 (Test FP01).

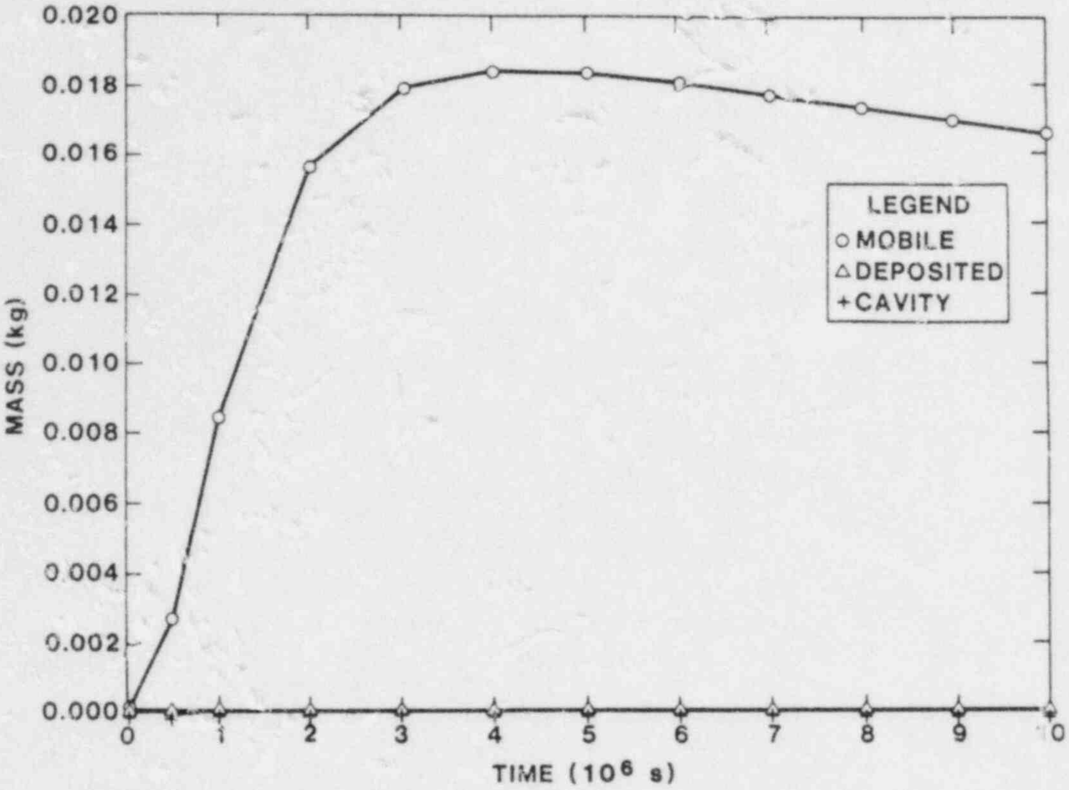

Figure FP-04 Decay of fission product DUM4 (Test FP01).

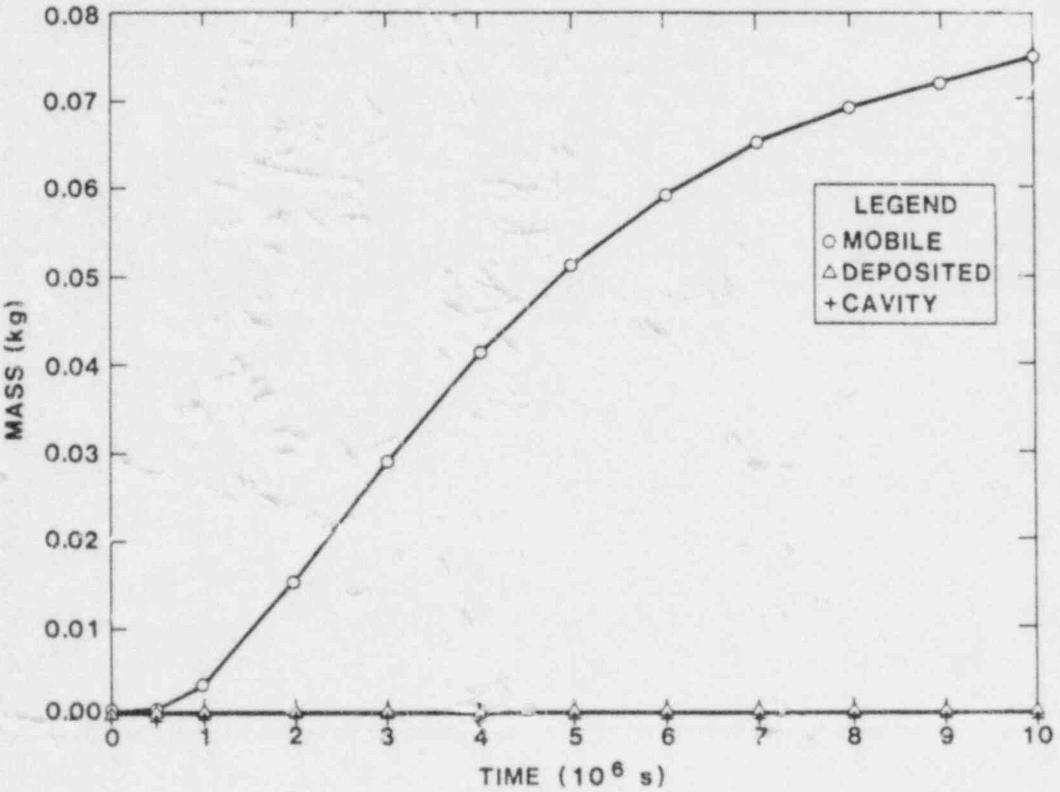

Figure FP-05 Decay of fission product DUM5 (Test FP01).

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FP02(ST) USER NAME: F. SCIACCA

2. TEST LEVEL: TL4A

3. TITLE OF TEST: TWO-ELEMENT FISSION-PRODUCT DECAY

4. CODE VERSION (DATE): 208 (2/10/82)

5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO STRUCTURES

7. TEST: SPECIFIED TWO, 2-ELEMENT DECAY CHAINS AND NO RELEASE. COMPARED RESULTS WITH EXACT ANALYTICAL SOLUTION.

8. RESULTS OF TEST: CONTAIN RESULTS WERE ESSENTIALLY IN COMPLETE AGREEMENT WITH THOSE OF THE EXACT ANALYTICAL SOLUTION. THE FISSION-PRODUCT MASSES PREDICTED BY CONTAIN FOR VARIOUS DECAY TIMES CLOSELY MATCHED THOSE PREDICTED BY THE ANALYTICAL SOLUTION.

	REMAINING MASS			
ELEMENT	TIME = 1.0E6 S		TIME = 10.0E6 S	
NAME	CALCULATED	CONTAIN	CALCULATED	CONTAIN
TE132	0.7814	0.7813	0.08473	0.08473
I132	0.02368	0.02368	0.00256	0.00256
I133	0.3963	0.3963	9.55E-5	9.546E-5
XE133	0.9834	0.9834	0.3722	0.3721

FIGURES FP-06 AND FP-07 SHOW THE DECAY OF TE132 AND I132, RESPECTIVELY. THE I132 DECAYS MUCH FASTER THAN THE TE132, AND ITS MASS DECREASES RATHER RAPIDLY EVEN THOUGH IT IS BEING PRODUCED BY THE TE132 DECAY. FIGURES FP-08 AND FP-09 SHOW THE CORRESPONDING RESPONSES FOR I133 AND XE133. IN THIS CASE THE DAUGHTER PRODUCT, XE133, HAS A LONGER HALF LIFE THAN THE PARENT, I133. THEREFORE, ITS MASS INCREASES UNTIL THE MASS OF I133 BECOMES SO LOW THAT THE PRODUCTION RATE OF XE133 FALLS BELOW ITS DECAY RATE.

9. COMMENTS: NONE

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

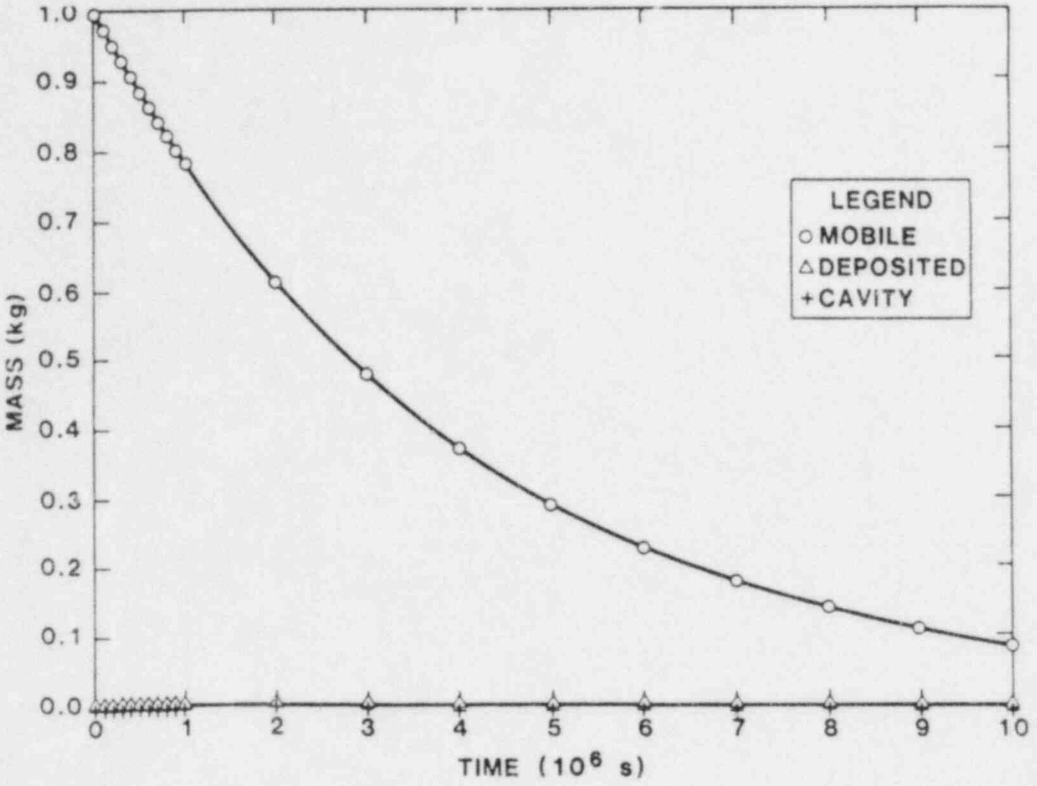

Figure FP-06 Decay of fission product TE132 (Test FP02).

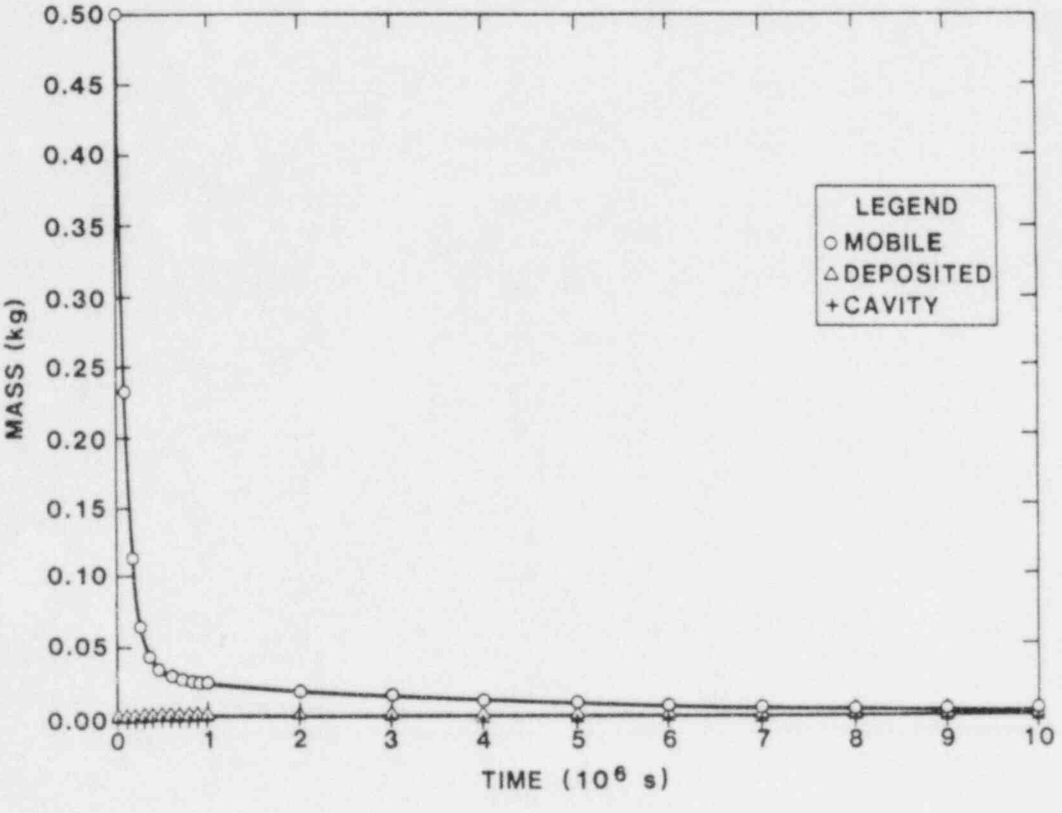

Figure FP-07 Decay of fission product I132 (Test FP02).

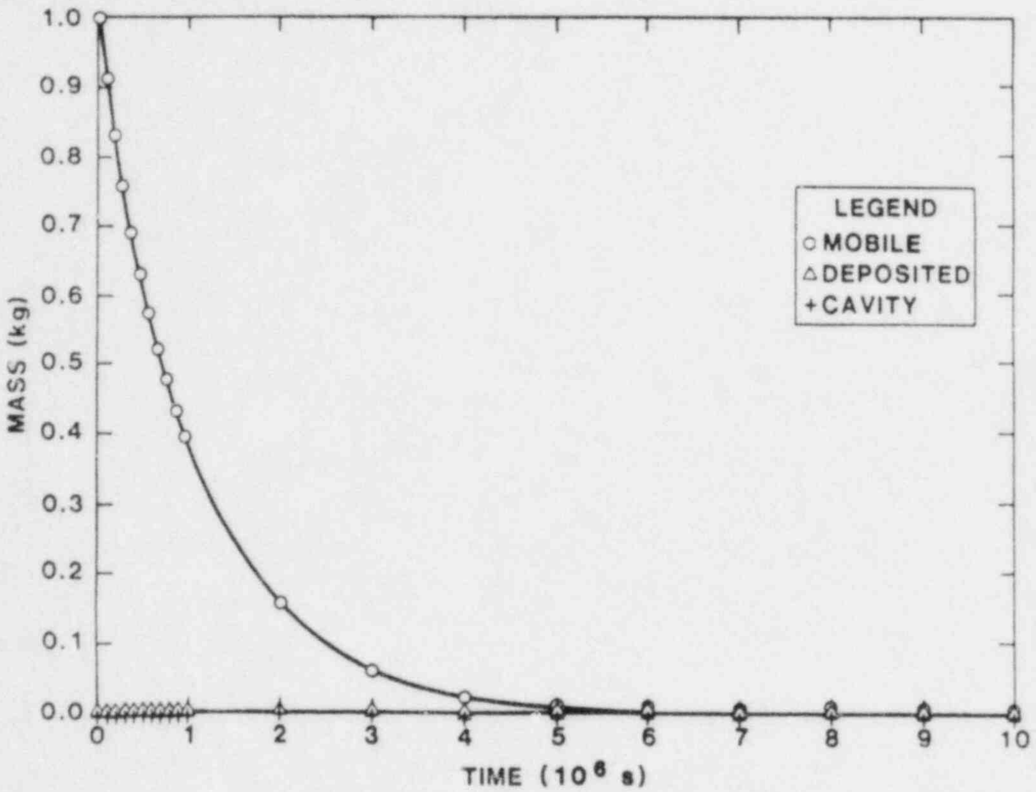

Figure FP-08 Decay of fission product I133 (Test FP02).

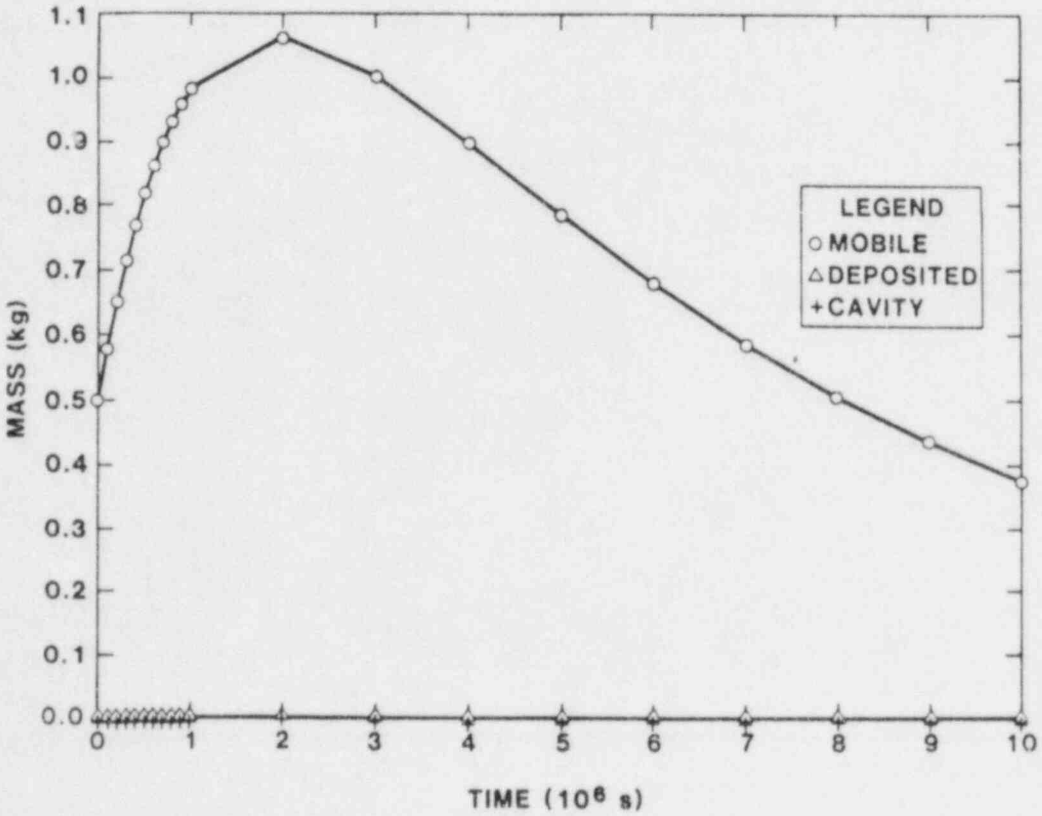

Figure FP-09 Decay of fission product XE133 (Test FP02).

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FP03 AND FP01 USER NAME: F. SCIACCA
2. TEST LEVEL: TL3
3. TITLE OF TEST: FISSION-PRODUCT DECAY: EFFECT OF PROBLEM TIME STEP
4. CODE VERSION (DATE): 208 (2/11,82)
5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY
6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO STRUCTURES AND NO SOURCES. SAME AS USED IN FP01.
7. TEST: USED SINGLE 5-ELEMENT DECAY CHAIN. ORIGINAL PARENT HAD A MUCH LONGER HALF-LIFE THAN THE IMMEDIATE DAUGHTER (IDENTICAL TO FP01). USED SINGLE LARGE TIME STEP (INSTEAD OF MANY STEPS AS WERE USED IN FP01) TO SEE IF SOLUTION SENSITIVE TO TIME-STEP SIZE.
8. RESULTS OF TEST: FP03 AND FP01 IN EXCELLENT AGREEMENT. RESULTS FOR THIS TYPE OF PROBLEM NOT SENSITIVE TO TIME-STEP SIZE.
9. COMMENTS: NONE
10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FP04 USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: FISSION-PRODUCT RELEASE AND ACCEPTANCE FUNCTIONS
4. CODE VERSION (DATE): 208 (2/11/82)
5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY, RELEASE AND ACCEPTANCE ROUTINES
6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO STRUCTURES AND NO SOURCES.
7. TEST: USED TWO, 2-ELEMENT FISSION-PRODUCT DECAY CHAINS; ALL FPS HAVE VERY SMALL DECAY RATES (LONG HALF-LIVES) COMPARED WITH RELEASE RATES. 1.0 KG OF EACH FISSION PRODUCT WAS SPECIFIED INITIALLY. DIFFERENT RELEASE RATES WERE SPECIFIED FOR EACH FISSION PRODUCT.

8. RESULTS OF TEST: CONTAIN RESULTS WERE COMPARED WITH THOSE FROM HAND CALCULATIONS. HAND CALCULATIONS IGNORED FP DECAY BECAUSE HALF-LIVES WERE LONG COMPARED WITH THE PROBLEM TIME. THE RESULTS WERE IN GENERALLY GOOD AGREEMENT, WITH ONLY A FRACTION OF A PERCENT DIFFERENCE BETWEEN THE TWO CALCULATIONS. CONTAIN PREDICTED SLIGHTLY LESS MASS PRESENT AT THE END OF EACH TIME STEP THAN DID THE HAND CALCULATION. THIS IS TO BE EXPECTED BECAUSE THE HAND CALCULATIONS IGNORED FP DECAY, WHEREAS CONTAIN TOOK THIS INTO ACCOUNT. THE FINAL DISTRIBUTION OF THE FISSION PRODUCTS AS INDICATED BY CONTAIN WAS IN AGREEMENT WITH EXPECTATIONS.

9. COMMENTS: NONE.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FP05 AND FP04 USER NAME: F. SCIACCA

2. TEST LEVEL: TL3

3. TITLE OF TEST: RELEASE AND ACCEPTANCE SENSITIVITY TO TIME-STEP SIZE

4. CODE VERSION (DATE): 208 (2/11/82)

5. ACTIVE MODULES OR OPTIONS: FISSION→PRODUCT DECAY, RELEASE AND ACCEPTANCE

6. CONTAINMENT CONFIGURATION AND SOURCES: SAME AS FP04--SINGLE CELL WITH NO STRUCTURES OR SOURCES.

7. TEST: TEST OF THE EFFECT OF PROBLEM TIME-STEP SIZE ON RELEASE AND ACCEPTANCE CALCULATIONS. USED FIVE LONG TIME STEPS RATHER THAN THE MANY SMALLER TIME STEPS USED IN FP04; OTHERWISE, SAME AS FP04.

8. RESULTS OF TEST: COMPARISON OF RESULTS OF TEST FP04 AND FP05 SHOWS THAN THE TIME-STEP SIZE DEFINITELY HAS AN EFFECT ON THE AMOUNT OF FISSION PRODUCTS RELEASED AND ACCEPTED. THE DISCREPANCIES IN THESE CALCULATIONS ARE GENERALLY QUITE SMALL (A FRACTION OF A %).

9. COMMENTS: IN GENERAL, TO AVOID INACCURACIES DUE TO EFFECTS OF TIME-STEP SIZE, TIME STEPS SHOULD BE SMALLER THAN A CHARACTERISTIC RELEASE TIME, I.E., THE RECIPROCAL OF THE LARGEST RELEASE RATE SPECIFIED FOR THE PROBLEM.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FP06(ST) USER NAME: F. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: TEST OF FP RELEASE AND ACCEPTANCE FUNCTIONS WITH DECAY RATES ON SAME ORDER AS RELEASE RATES
4. CODE VERSION (DATE): 208 (2/11/82)
5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY, RELEASE, AND ACCEPTANCE
6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO STRUCTURES OR SOURCES
7. TEST: USED TWO, 2-ELEMENT FISSION-PRODUCT DECAY CHAINS. RELEASE RATES SPECIFIED AS SAME ORDER AS FP DECAY RATES. COMPARED CONTAIN RESULTS WITH RESULTS OF SEPARATE ANALYTICAL SOLUTION.
8. RESULTS OF TEST: CONTAIN RESULTS AGREE CLOSELY WITH RESULTS OF SEPARATE ANALYTICAL SOLUTION. SAMPLE RESULTS ARE GIVEN IN THE FOLLOWING TABLE.

	MASS REMAINING IN ORIGINAL HOST			
ELEMENT	TIME = 50.0 S		TIME = 200.0 S	
NAME	CALCULATED	CONTAIN	CALCULATED	CONTAIN
TE132	6.580E-6	6.580E-6	1.88E-21	1.87E-21
I132	0.7998	0.7998	0.06310	0.06309
I133	0.9479	0.9479	0.80746	0.80750
XE133	0.9693	0.9693	0.8825	0.8825

9. COMMENTS: NONE
10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FP08 AND FP07 USER NAME: F. SCIACCA
2. TEST LEVEL: TL3
3. TITLE OF TEST: CHECK OF TIME-STEP SENSITIVITY ON FISSION-PRODUCT RELEASE AND DECAY
4. CODE VERSION (DATE): 208 (2/12/82)
5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY AND RELEASE/ACCEPTANCE
6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO STRUCTURES OR SOURCES

7. TEST: USED TWO, 2-ELEMENT FISSION-PRODUCT DECAY CHAINS AS IN FP06. RELEASE RATES ON SAME ORDER AS DECAY RATES. FP07 USED A SINGLE LONG TIME STEP, FP08 USED A FEW LONG TIME STEPS. CHECKED ON SENSITIVITY OF RESULTS TO TIME-STEP SIZE AND COMPARED WITH RESULTS FROM FP06.

8. RESULTS OF TEST: FOR FP07 WITH A SINGLE LONG TIME STEP, NOT ALL OF THE FISSION PRODUCTS GOT DISTRIBUTED. FOR FP08 SOME OF THE DISTRIBUTED MASSES EXACTLY MATCHED THE RESULTS FROM FP06. FOR OTHERS, DIFFERENCES ON THE ORDER OF 3% RELATIVE TO FP06 RESULTS WERE NOTED.

9. COMMENTS: TIME-STEP SIZE WILL HAVE SOME EFFECT ON FISSION-PRODUCT DISTRIBUTED MASSES. EFFECT IS NOT VERY LARGE EXCEPT FOR TIME STEPS LONG COMPARED WITH RELEASE TIMES. TIME STEPS SHOULD BE KEPT SHORT RELATIVE TO A CHARACTERISTIC RELEASE TIME (SEE REPORT FOR FP05).

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FP09 USER NAME: F. SCIACCA

2. TEST LEVEL: TL3

3. TITLE OF TEST: CHECK OF RELEASE AND ACCEPTANCE ON TOTAL MASS OF EACH ELEMENT OF A 5-ELEMENT DECAY CHAIN

4. CODE VERSION (DATE): 208 (2/15/82)

5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY AND RELEASE/ACCEPTANCE

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE CELL WITH NO STRUCTURES OR SOURCES

7. TEST: CHECK OF EFFECT OF RELEASE AND ACCEPTANCE ON MASS CONSERVATION OF EACH FISSION PRODUCT OF A MULTIELEMENT CHAIN. COMPARED RESULTS WITH THOSE FROM FP01. USED SAME 5-ELEMENT DECAY CHAIN AS USED IN FP01, BUT SPECIFIED RELEASE AND ACCEPTANCE PARAMETERS.

8. RESULTS OF TEST: MASSES FROM FP09 (WITH RELEASE) ARE EXACTLY THE SAME AS THE MASSES FROM FP01. THEREFORE, RELEASE AND ACCEPTANCE OF FISSION PRODUCTS DO NOT AFFECT MASS CONSERVATION OF ELEMENTS TRANSFERRED.

9. COMMENTS: NONE.

10. SUGGESTIONS FOR ADDITIONAL TESTS: CHECK INTERCELL FLOW OF FISSION PRODUCTS.

Supporting Analysis: FP Series - Fission-Product Decay and Release

A. Decay of Multi-Element Chain with Half-Life of Initial Parent Very Long Compared to Half-Life of Immediate Daughter Product:

The equation for the generation rate of the immediate daughter product is as follows:

$$\frac{dN_2}{dt} = \lambda_1 N_1 - \lambda_2 N_2 \tag{3.4-1}$$

where

λ_n = decay constant of fission product n

N_n = number of atoms of fission product n

If the half-life of the parent, $(\Theta_{1/2})_1$, is much longer than that of the immediate daughter, $(\Theta_{1/2})_2$, then $\lambda_1 << \lambda_2$. Then after some time, N_2 becomes approximately fixed so that

$$\frac{dN_2}{dt} = 0 \tag{3.4-2}$$

$$\lambda_1 N_1 \simeq \lambda_2 N_2 \tag{3.4-3}$$

At this stage N_2 behaves like an isotope with a very long half-life, so that at late times

$$\lambda_2 N_2 \simeq \lambda_3 N_3 \ . \tag{3.4-4}$$

Eventually,

$$\lambda_1 N_1 \simeq \lambda_2 N_2 \simeq \lambda_3 N_3 \simeq \lambda_4 N_4 \simeq \lambda_n N_n \tag{3.4-5}$$

Note that $N_1 = N_{1_o} e^{-\lambda_1 t}$ (number of atoms)

where N_{1_o} = number of atoms of element 1 present at t = 0

Also, $M_1 = M_{1_o} e^{-\lambda_1 t}$ (mass of element 1). Therefore

$$M_n \simeq \left[M_{1_o} e^{-\lambda_1 t} \ \frac{\lambda_1}{\lambda_n} \right] \tag{3.4-6}$$

This approximate solution gives good results for cases where $t >> (\Theta_{1/2})_1$.

B. Decay of Two-Element Fission-Product Chain:

For the case of a two-element fission-product decay chain, the amount of each element present at any time can be solved for exactly:

$$N_1 = N_{1_o} e^{-\lambda_1 t} \tag{3.4-7}$$

$$N_2 = \frac{\lambda_1 N_{1_o}}{\lambda_2 - \lambda_1}\left[e^{-\lambda_1 t} - e^{-\lambda_2 t}\right] + N_{2_o} e^{-\lambda_2 t} \tag{3.4-8}$$

In terms of the masses, note that the molecular weights of both isotopes are approximately equal and therefore

$$M_1 = M_{1_o} e^{-\lambda_1 t} \tag{3.4-9}$$

$$M_2 = \frac{\lambda_1 M_{1_o}}{\lambda_2 - \lambda_1}\left[e^{-\lambda_1 t} - e^{-\lambda_2 t}\right] + M_{2_o} e^{-\lambda_2 t} \tag{3.4-10}$$

where M_{1_o}, M_{2_o} = mass of each isotope at $t = 0$

C. Fission-Product Release and Acceptance:

In CONTAIN, fission products can be released from one host material and accepted by other host materials. The release from a host is assumed to be exponential in nature. The fraction released in a given time step is represented by the following equation:

$$R = 1-e^{-r\Delta t} \tag{3.4-11}$$

where

R = fraction of the isotope in the host which is released in time step Δt

r = release rate, s^{-1}

The fraction of the isotope remaining in the host following the release is simply

$$S = e^{-r\Delta t} \tag{3.4-12}$$

Thus, the amount of isotope i remaining in the original host at the end of a time step is expressed as follows:

$$M_{i(after)} = M_{i(before)} e^{-r\Delta t} \tag{3.4-13}$$

where $M_{i(before)}$ is calculated according to equation (3.4-9) and (3.4-10) for isotopes in a two-element decay chain.

CONTAIN's treatment of fission-product acceptance was checked qualitatively rather than quantitatively.

SERIES FP STANDARD TEST INPUT DATA SETS

```
&&      ------------------------ FP02(ST) ------------------------------------

CONTROL=9 1 2 2 4 2 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL
FISSION
TE132 I132
I133 XE133
TIMES 50.0 0.0 1.0E4 1.0E4 1.0E5 1.0E5 1.0E5 1.0E6 1.0
PRFISS
FISSION 0 2 2
TE132 I132
I133 XE133
2.808E5 8.226E3
7.488E4 4.571E5
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 0.5 1.0 0.5
EOI
TITLE
    FISSION PRODUCT DECAY CHAIN TEST
  CASE FP02(ST): 2-ELEMENT DECAY CHAINS WITH ARBITRARY DECAY CONSTANTS
FAST
CELL =1
CONTROL=18 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
GEOMETRY 100.0 10.0
ATMOS=2
1.013E5  300.0
N2=0.78
O2=0.22
EOF
```

```
&&      ---------------------- FP06(ST) ---------------------------------------

CONTROL=9 1 3 3 4 2 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL
FISSION
TE132 I132
I133 XE133
TIMES 50.0 0.0 10.0 10.0 1.0E2 1.0E2 1.0E3 1.0E3 1.0E3 1.0E3 5.0E3 1.0
PRFISS
FISSION 0 2 2
TE132 I132
I133 XE133
5.0 100.0
1.0E4 1.0E3
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 1.0 1.0
```

```
RELEASE
TE132 1.0E-1
I132  1.0E-2
I133  1.0E-3
EOI
ACCEPT
TE132 0 0 0.5 0.5
I132 0 0  0.5 0.5
I133  0 0 0.25 0.75
EOI
EOI
TITLE
     FISSION PRODUCT DECAY CHAIN TEST
 CASE FP06(ST): TEST OF RELEASE AND ACCEPTANCE FUNCTIONS
RELEASE RATES ON THE SAME ORDER AS FP HALF-LIVES
FAST
CELL =1
CONTROL=18 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
GEOMETRY 100.0 10.0
ATMOS=2
1.013E5  300.0
N2=0.78
O2=0.22
EOF
```

3.4.2 Series FT - Fission-Product Intercell Transport

The CONTAIN treatment of fission products allows for their transport from one cell to another. This movement is accomplished via the intercell flow of suitable host materials. In test FT01, four fission products in two decay chains were used. The isotopes of chain 1 were attached to the gas in cell 1 as their host material. For chain 2, a selected aerosol was the host. The test provided for flow of these host materials from cell 1 to cell 2. The test results indicate that CONTAIN's treatment of fission-product intercell transport is quite good, at least for two-cell systems.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FT01(ST) USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: FISSION-PRODUCT INTERCELL TRANSPORT
4. CODE VERSION (DATE): 705(1983) 10-16-83
5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY, FLOWS, HEAT TRANSFER
6. CONTAINMENT CONFIGURATION AND SOURCES: USED A TWO-CELL ARRANGEMENT SIMILAR TO THAT USED IN TEST CF04. THE TWO CELLS ARE INTERCONNECTED AND CONTAIN HEAT SINKS TO MAINTAIN NEAR-ISOTHERMAL CONDITIONS. CELL 1 IS INITIALLY AT A HIGHER PRESSURE THAN CELL 2. FOUR FISSION PRODUCTS IN TWO CHAINS ARE USED. THE CELL GAS IS THE HOST FOR THE FISSION PRODUCTS IN CHAIN 1. THE AEROSOL NA2O2 IS THE HOST FOR ISOTOPES IN CHAIN 2. ALL THE FISSION PRODUCTS AND AEROSOLS ARE INITIALLY IN CELL 1.
7. TEST: COMPARE THE CONTAIN PREDICTIONS OF FISSION-PRODUCT MASSES IN EACH CELL VS TIME WITH PREDICTIONS FROM HAND CALCULATIONS.
8. RESULTS OF TEST: THE CONTAIN RESULTS AND THOSE FROM THE HAND ANALYSIS WERE IN EXCELLENT AGREEMENT. THE INITIAL CONDITIONS FOR THE FISSION PRODUCTS WERE AS FOLLOWS:

NAME	CHAIN	MASS	HOST	HALF LIFE
DUM1	1	1.0	GAS	1.0E4 SEC
DUM2	1	1.0	GAS	0.9E4
DUM3	2	1.0	NA2O2(AER)	1.1E4
DUM4	2	1.0	NA2O2(AER)	1.0E2

SAMPLE COMPARISONS OF THE CONTAIN VS CALCULATED RESULTS FOR THIS TEST ARE AS FOLLOWS:

	MASS OF FISSION PRODUCT IN CELL 2			
NAME	TIME = 30 S		TIME = 60 S	
	CALCULATED	CONTAIN	CALCULATED	CONTAIN
DUM1	0.02902	0.02904	0.04324	0.04325
DUM2	0.02908	0.02909	0.04340	0.04341
DUM3	0.02877	0.02876	0.04256	0.04258
DUM4	0.02346	0.02346	0.02832	0.02833

NAME	TIME = 90 S		TIME = 500 S	
	CALCULATED	CONTAIN	CALCULATED	CONTAIN
DUM1	0.04515	0.04517	0.04388	0.04390
DUM2	0.04540	0.04542	0.04523	0.04525
DUM3	0.04445	0.04442	0.04326	0.04328
DUM4	0.02414	0.02413	0.00178	0.00178

THE INITIAL PRESSURE DIFFERENTIAL BETWEEN THE TWO CELLS WAS QUITE SMALL, AND THE TOTAL MASS TRANSFERRED FROM CELL 1 TO CELL 2 WAS ONLY ABOUT 5% OF THE INITIAL MASS IN CELL 1. HENCE, ONLY A SMALL AMOUNT OF FISSION-PRODUCT MASS WAS TRANSFERRED.

THIS TEST CLEARLY DEMONSTRATES THAT CONTAIN DOES PROVIDE FOR THE TRANSPORT OF FISSION PRODUCTS FROM ONE CELL TO ANOTHER. BOTH GAS AND AEROSOL HOSTS CAN BE USED FOR THIS TRANSPORT.

FIGURES FT-01 AND FT-02 SHOW THE MASS OF EACH FISSION PRODUCT IN CELL 1 AS A FUNCTION OF TIME AS PREDICTED BY CONTAIN. IN FIGURE FT-01, THE MASS OF DUM2 IS GREATER THAN THAT OF DUM1 BECAUSE DUM1 DECAYS TO DUM2. FIGURE FT-02 SHOWS THAT SOME DUM3 AND DUM4 HAS BEEN DEPOSITED AS A RESULT OF THEIR HOST AEROSOL'S SETTLING OUT WITH TIME. FISSION PRODUCT DUM4 HAD A RELATIVELY SHORT HALF LIFE, AND ITS MASS DECREASES RATHER RAPIDLY. FIGURES FT-03 AND FT-04 SHOW THE FISSION-PRODUCT MASSES IN CELL 2 VS TIME. ALL OF THE TRENDS DISPLAYED IN THESE FIGURES ARE QUALITATIVELY AND QUANTITATIVELY AS EXPECTED.

9. COMMENTS: THE HAND ANALYSIS PERFORMED IN SUPPORT OF THIS TEST UTILIZED THE CONTAIN RESULTS FOR GAS AND AEROSOL MASSES FLOWING FROM CELL 1 TO CELL 2. THE FISSION-PRODUCT TRANSPORT WAS THEN CALCULATED ASSUMING THAT IT WAS STRICTLY PROPORTIONAL TO THE FLOW OF THE HOST MATERIAL. FISSION-PRODUCT DECAY WAS TAKEN INTO ACCOUNT.

   IN SETTING UP THIS TEST DATA SET, A PROBLEM WAS ENCOUNTERED WHEN THE TWO ISOTOPES IN A DECAY CHAIN WERE GIVEN THE SAME HALF LIFE. CURRENTLY, CONTAIN CANNOT HANDLE THIS SITUATION. THE CODE WILL ABORT IF TWO CONSECUTIVE FISSION PRODUCTS IN THE SAME CHAIN HAVE IDENTICAL HALF LIVES. HOWEVER, THIS SHOULD NOT POSE ANY REAL RESTRICTIONS FOR MOST PRACTICAL PROBLEMS.

10. SUGGESTIONS FOR ADDITIONAL TESTS: TESTS OF FISSION-PRODUCT TRANSPORT IN PARALLEL FLOW PATHS AND IN CASES WITH MORE THAN TWO CELLS IN SERIES.

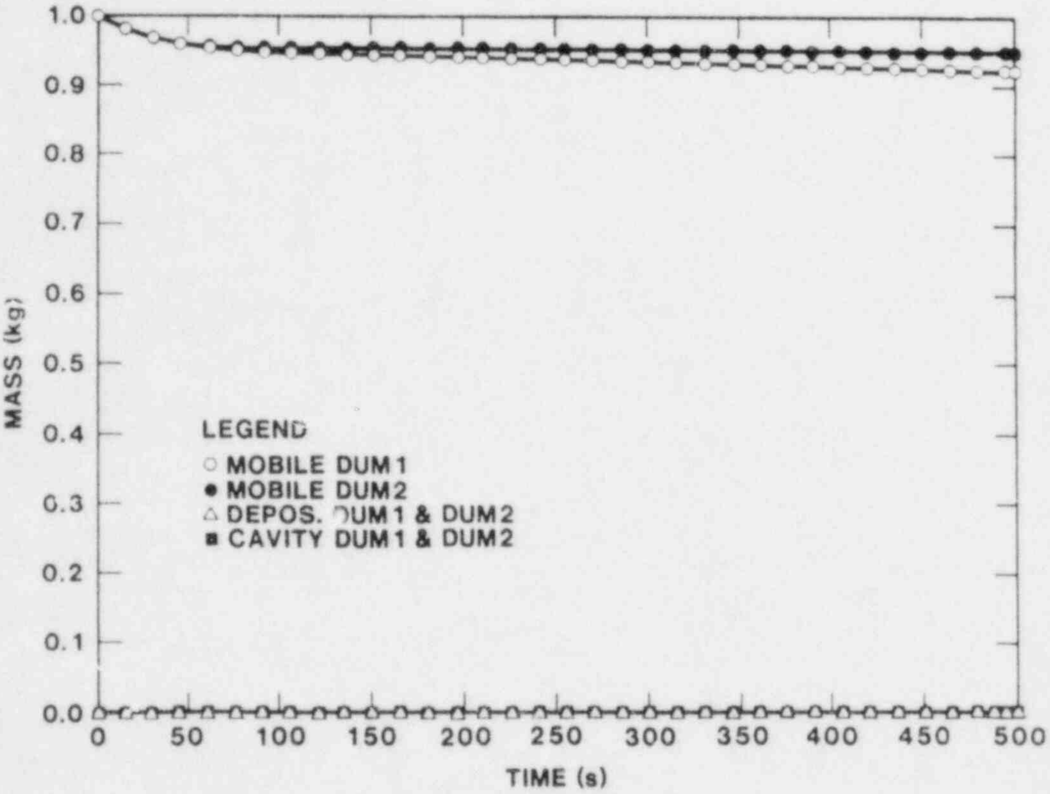

Figure FT-01 Mass of fission products DUM1 and DUM2 in Cell 1.

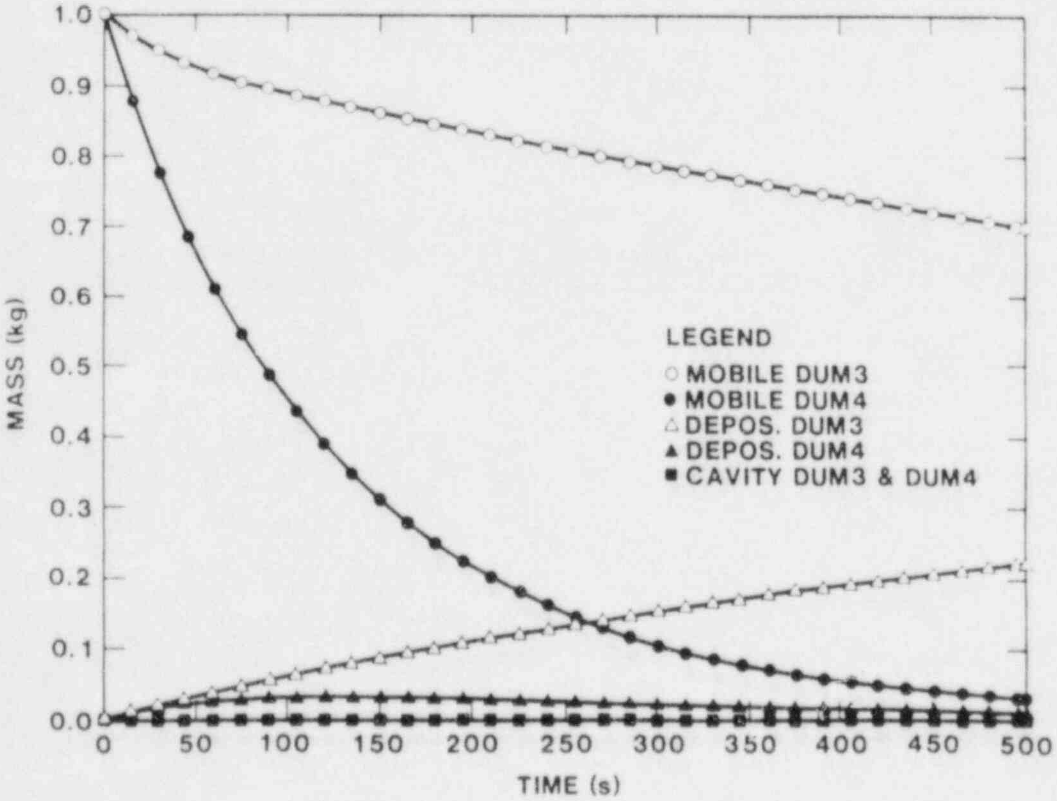

Figure FT-02 Mass of fission products DUM3 and DUM4 in Cell 1.

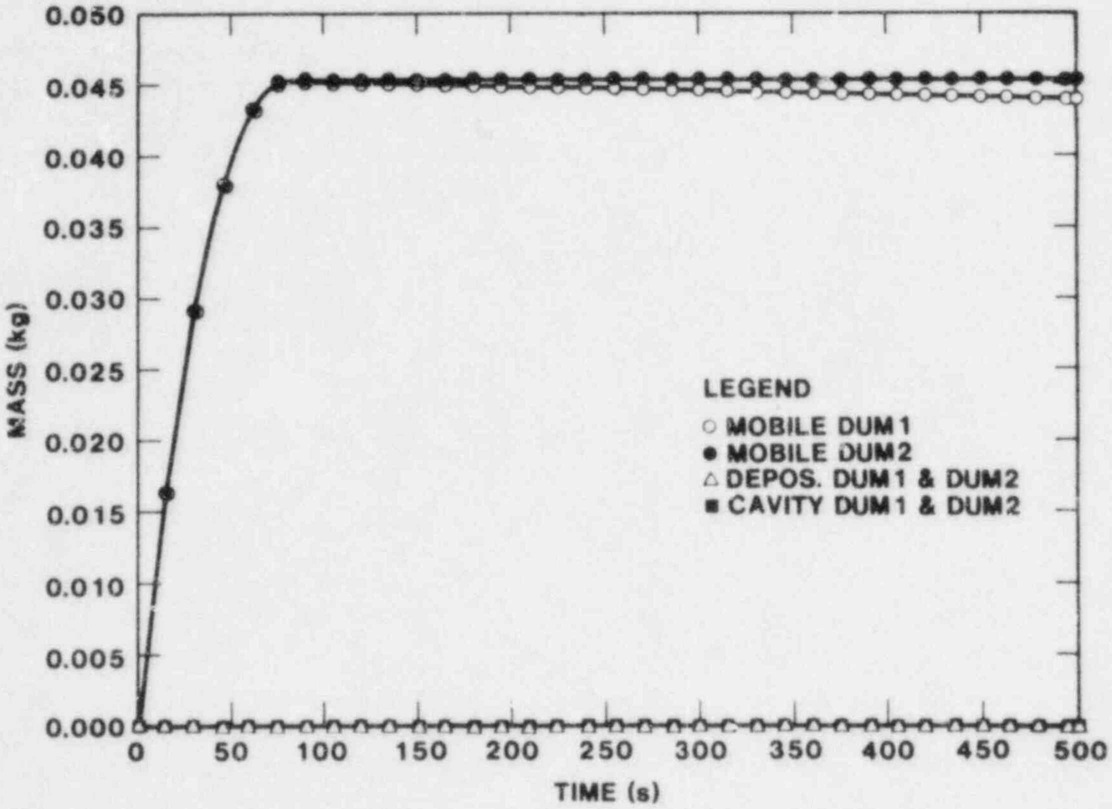

Figure FT-03 Mass of fission products DUM1 and DUM2 transported into Cell 2.

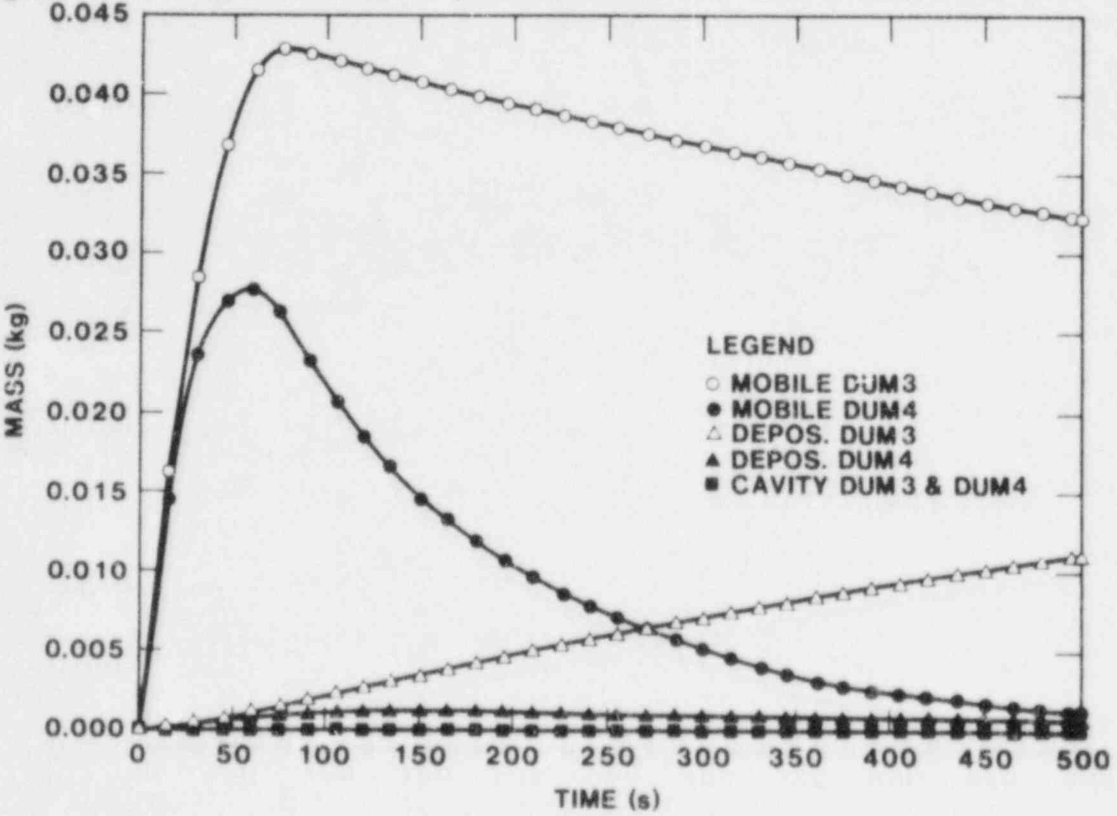

Figure FT-04 Mass of fission products DUM3 and DUM4 transported into Cell 2.

Supporting Analysis: FT Series - Fission-Product Intercell Transport

The mass of fission product transported with a host material is assumed to be proportional to the mass of the host material that has flowed from one cell to another. The mass of the fission product remaining in the first cell is then given by:

$$M_{FP_{i,t}} = M_{FP_{i,t-1}} \left[\frac{M_{H,t}}{M_{H,t-1}} \right] \qquad (3.4\text{-}14)$$

where

$M_{FP_{i,t}}$ = mass of FP_i in cell 1 at end of current time step

$M_{FP_{i,t-1}}$ = mass of FP_i in cell 1 at end of previous time step

$M_{H,t}$ = mass of host material in cell 1 at end of current time step

$M_{H,t-1}$ = mass of host material in cell 1 at end of previous time step

Once the flow has taken place, the fission-product decay is taken into account using equation (3.4-9) or (3.4-10), depending on whether the first or second element in the decay chain is being treated. The M_{1_o} and M_{2_o} in these equations become $M_{FP_{1,t}}$ and $M_{FP_{2,t}}$, respectively, for use in equation (3.4-14). A stepwise process is used to calculate the masses of each fission product as a function of time.

The mass of the host material in cell 1 versus time, as used in equation (3.4-14), was taken from the CONTAIN output.

The mass of fission products in cell 2 versus time is calculated by first noting the total mass of each fission product present in the system and subtracting from this the mass in cell 1.

SERIES FT STANDARD TEST INPUT DATA SET

```
&& --------------FT01(ST)-----------------------------------------------------

CONTROL = 9 2 4 1 4 2 20 2 0 0
MATERIAL
COMPOUND N2 02 H2 HE NAV NAL FE NA20 NA202
FISSION
DUM1 DUM2
DUM3 DUM4
TIMES 50.0 0.0 1.0 15.0 500.1 1.0 1.0
FLOWS
  AREA(1.2)=0.020 AVL(1,2)=0.05  CFC(1,2)=2.0 TOPEN(1.2)=0.0 QUASI
PRFISS PRFLOW PRAER
FISSION 0 0 2 2
DUM1 DUM2
DUM3 DUM4
1.0E4 0.9E4
1.1E4 1.0E2
1.0 1.0 1.0 1.0
FPM-CELL=1
HOST=GAS 1.0 1.0 0.0 0.0
HOST=AEROSOL 2 0.0 0.0 1.0 1.0
EOI
AEROSOL 0 0 0 0 0 0 0 NA20 =2.0E-6 0.0 NA202=1.0E-6 0.0
TITLE
     TEST OF FISSION PRODUCT TRANSPORT.  VERSION 705.
   CASE FT01(ST):  INITIAL CONCENTRATION OF 1000 MG/M**3 IN CELL #1
    QUASI-STEADY FLOW BETWEEN CELLS.  CELL FLOW SETUP SIMILAR TO CASE CF04.
     SAME AS CASE AF04 EXCEPT TWO AEROSOL COMPONENTS & ONE AER AS FP HOST.
FAST

CELL=1
CONTROL=17 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
   HIGH PRESSURE CELL (#1)
GEOMETRY
1000.0 10.0
ATMOS=1
1.1E5 300.0
N2 1.0
&& ------------------ LARGE HEAT SINK ----------------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 1 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
   FE  FE  FE
AEROSOL=2 NA20 1.0 NA202 1.0
CELL = 2
CONTROL=17 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
   LOW PRESSURE CELL (#2)
GEOMETRY
```

```
1000.0 10.0
ATMOS=1
1.0E5 300.0
N2 1.0
&& -------------------CELL #2 HEAT SINK ----------------------------------------
STRUC
   HEATSINK
   WALL
   SLAB 3 2 300.0 1.0 0 1.0E5
   0.0 0.005 0.010 0.015
   FE FE FE
EOF
EOI
```

3.4.3 Series FH - Fission-Product Heating of Structures

In this test series, CONTAIN's treatment of fission-product heating of structures was investigated. This heating occurs when fission products are plated out on surfaces of structures. The tests used an insulated slab to model both a floor structure and a wall structure. The only heat transfer to or from the slab was that due to fission-product heating. Two different slab materials were used in the tests.

The testing revealed a problem in CONTAIN's treatment of fission-product heating of walls that had both right and left faces enclosed in the same cell; only half of the available decay heat was applied. A modest coding change was identified to correct this problem. The code's treatment of floor and roof structures was sound, and no corrections were needed.

With the minor correction noted above, CONTAIN's treatment of fission-product heating of structures appears to be satisfactory.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: FH01 THROUGH FH05(ST), FH06 USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: FISSION-PRODUCT HEATING OF STRUCTURES
4. CODE VERSION (DATE): 705(83) 10-18-83
5. ACTIVE MODULES OR OPTIONS: FISSION-PRODUCT DECAY, STRUCTURE HEAT TRANSFER.
6. CONTAINMENT CONFIGURATION AND SOURCES: USED A SINGLE CELL CONTAINING A SINGLE HEAT STRUCTURE. THE STRUCTURE IS TOTALLY ENCLOSED WITHIN THIS CELL. A FISSION PRODUCT WITH A SIGNIFICANT DECAY HEAT IS PRESENT ON THE STRUCTURE. ALL OTHER HEAT TRANSFER IS TURNED OFF. TWO DIFFERENT STRUCTURE MATERIALS WERE USED IN THE VARIOUS TESTS.
7. TEST: COMPARE THE STRUCTURE TEMPERATURES AS CALCULATED BY CONTAIN WITH THOSE GENERATED BY HAND ANALYSIS.
8. RESULTS OF TEST: TWO TYPES OF STRUCTURES WERE USED, A FLOOR AND A WALL. THE DIFFERENT MATERIALS USED WERE FE AND NAOH. THE FE AS USED IN CONTAIN HAS A SPECIFIC HEAT WHICH VARIES WITH TEMPERATURE, WHILE THE NAOH HAS A CONSTANT SPECIFIC HEAT. THE FOLLOWING TABLE GIVES THE MAJOR TEST VARIABLES AND THE KEY RESULTS.

TEST	STRUC TYPE	MATL	HALF-LIFE	STRUC TEMP @ 10000 S, K CALC	CONTAIN
FH01	WALL	FE	1.0E4	1577	860
FH02	WALL	FE	1.0E8	2070	1056
FH03	FLOOR	FE	1.0E4	1334	1345
FH04	FLOOR	FE	1.0E8	1734	1646
FH05	FLOOR	NAOH	1.0E8	3145	3144
FH06	FLOOR	NAOH	5.0E3	1840	1843

THESE RESULTS REVEALED A PROBLEM WITH THE CONTAIN TREATMENT OF FISSION-PRODUCT HEATING OF WALLS LOCATED ENTIRELY WITHIN ONE CELL. THE CODE WAS PROVIDING ONLY HALF OF THE INTENDED AMOUNT OF HEATING TO SUCH STRUCTURES. AN UPDATE WAS IDENTIFIED TO CORRECT THIS ERROR. THIS PROBLEM DID NOT EXIST FOR FLOORS OR ROOFS.

GOOD AGREEMENT BETWEEN THE HAND CALCULATIONS AND THE CONTAIN PREDICTIONS OF STRUCTURE TEMPERATURES WAS ACHIEVED FOR THE CASES USING CONSTANT SPECIFIC HEAT MATERIALS (CASES FH05 AND FH06). ALL OF THE HAND CALCULATIONS ASSUMED A CONSTANT SPECIFIC HEAT FOR THE STRUCTURE MATERIALS. THIS USAGE UNDOUBTEDLY INTRODUCED SOME ERROR INTO THE HAND-ANALYSIS RESULTS.

9. <u>COMMENTS</u>: OVERALL, IT APPEARS THAT THE CONTAIN TREATMENT OF FISSION PRODUCT HEATING OF STRUCTURES IS REASONABLY SOUND, PROVIDING THAT THE PROBLEM WITH THE CODING FOR "WALL" STRUCTURES IS CORRECTED.

   THE CONTAIN RESULTS SHOW A TEMPERATURE GRADIENT THROUGH THE STRUCTURES. THE TEMPERATURE IS HIGHER ON THE LEFT FACE THAN IT IS ON THE RIGHT FACE. FOR THE CONDITIONS OF THESE TESTS (WITH BOTH FACES OF THE STRUCTURE WITHIN THE CELL), ONE WOULD EXPECT IDENTICAL FACE TEMPERATURES WITH A PARABOLIC TEMPERATURE PROFILE THROUGH THE STRUCTURE. THE CAUSE OF THIS PROBLEM HAS NOT YET BEEN INVESTIGATED.

   THE TESTS REPORTED HERE (FH01 THROUGH FH06) TREATED FISSION-PRODUCT HEATING OF STRUCTURES. FISSION-PRODUCT HEATING OF POOLS HAS ALSO BEEN TESTED AND IS DISCUSSED IN THE POOL-BOILING TEST SERIES (SERIES PB). CODE VERSIONS 501 AND BEYOND CORRECTLY PREDICT POOL HEATUP AND BOILING AS A RESULT OF FISSION-PRODUCT DECAY HEATING.

10. <u>SUGGESTIONS FOR ADDITIONAL TESTS</u>: TEST FP HEATING OF STRUCTURE WHOSE RIGHT FACE IS EITHER INSULATED OR WHICH SEES OTHER RIGHT-FACE CONDITIONS.

---

1. PROBLEM: ID NO. FP001 2. LEVEL: PL3 3. RESOLVED? YES
4. DESCRIPTION: THE CODE DID NOT PUT IN THE RIGHT AMOUNT OF DECAY HEAT FOR WALL STRUCTURES WITH BOTH FACES WITHIN ONE CELL.
5. DATE PROBLEM RESOLVED: 10-18-83

* * *

1. PROBLEM: ID NO. FP-02 2. LEVEL: PL2 3. RESOLVED? NO
4. DESCRIPTION: THE TEMPERATURE PROFILES FOR STRUCTURES WITH BOTH FACES HEATED BY FISSION PRODUCTS (SUPPOSEDLY EQUAL HEATING OF EACH FACE) ARE NOT AS ONE WOULD EXPECT.
5. DATE PROBLEM RESOLVED.

Supporting Analysis: Series FH - Fission-Product Heating of Structures

A slab with fission products on its outside surfaces is heated by the fission-product decay heat. The slab is insulated and does not transfer heat to or from the atmosphere or other objects. Find the slab temperture after a given period of heating.

The heat balance is

$$Q_{in} - Q_{out} = \text{change in stored heat}$$

$$= Q_f - Q_i$$

$$Q_{in} = \dot{Q}\Delta t$$

$$Q_{out} = 0$$

$$Q_f = m_s C_p T_f$$

$$Q_i = m_s C_p T_i$$

where $\dot{Q}$ = the rate of production of fission-product decay heat (in kJ/s), Δt = elapsed time, the subscript f means final, the subscript i means initial, m_s is the mass of the slab and C_p is its mean heat capacity (specific heat at constant pressure) over the temperature range T_i to T_f.

Therefore,

$$\dot{Q}\Delta t = m_s C_p (T_f - T_i) \qquad (3.4\text{-}15)$$

For the case where the fission-product decay heat changes significantly with time:

$$\dot{Q} = \dot{q}m = \dot{q}m_o e^{-\lambda t}$$

where $\dot{q}$ is the rate of production of heat per unit of fission-product mass, and m_o is the mass of the fission product at t = 0.

$$Q = \dot{Q}\Delta t = \int_0^t \dot{q}m_o e^{-\lambda t} dt$$

or

$$Q = \frac{\dot{q}m_o}{\lambda} (1 - e^{-\lambda t}) \qquad (3.4\text{-}16)$$

Combining equations (3.4-15) and (3.4-16),

$$T_f = T_i + \frac{\dot{q} m_o (1 - e^{-\lambda t})}{\lambda m_s C_p} \qquad (3.4\text{-}17)$$

SERIES FH STANDARD TEST INPUT DATA SET

```
&& ------------------FH05(ST)-----------------------------------------------------
CONTROL = 9 1 2 2 2 1 20 0 0 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL NAOH
FISSION
DUM1 DUM2
TIMES 50.0 0.0 25.0 200.0 1.0E3 50.0 200.0 1.0E4 1.0

PRFISS
PRHEAT
FISSION 0 2
DUM1 DUM2
1.0E8 1.0E5
1.0E3 1.0
FPM-CELL=1
HOST=FLOOR 10.0 0.0
EOI
TITLE
     FISSION PRODUCT DECAY HEATING TEST.  CONSTANT DECAY HEAT.
    CASE FH05(ST):  FISSION PRODUCT HEATING OF A NAOH SLAB FLOOR.  OTHER HT OFF.
FAST
CELL =1
CONTROL=17 0 0 1 3 0 0 0 0 0 0 0 0 0 0 0 0
GEOMETRY 100.0 10.0
ATMOS=2
1.013E5  300.0
N2=0.78
O2=0.22
STRUC
   HEATSINK
   FLOOR
   SLAB 3 1 300.0 1.0 0 1.0
   0.0 0.005 0.010 0.015
   NAOH NAOH NAOH
HT-TRAN OFF OFF OFF OFF OFF OFF OFF
EOF
 EOI
```

3.5 POOL THERMODYNAMICS AND HEAT TRANSFER

3.5.1 Series PQ - Pool-to-Atmosphere Heat Transfer

In this test series the heat transfer between a sodium pool and the atmosphere above it was checked. Specifically, the heat balance was checked. These tests revealed problems with the heat balance (versions 809 and earlier). Checks of the coding indicated an inconsistency in the units used in the atmosphere and pool routines. In addition, an initialization error was detected. These problems were corrected with appropriate updates.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: PQ03 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A

3. TITLE OF TEST: POOL-TO-ATMOSPHERE HEAT TRANSFER

4. CODE VERSION (DATE): 809 (9-1/15-82) AND 915 (9-17,20-82)

5. ACTIVE MODULES OR OPTIONS: POOL AND ATMOSPHERE THERMODYNAMICS, POOL-TO-ATMOSPHERE HEAT TRANSFER

6. CONTAINMENT CONFIGURATION AND SOURCES: A SINGLE LARGE CELL WAS MODELED. ITS VOLUME WAS 10000 M**3, ITS ATMOSPHERE WAS AIR AT AN INITIAL TEMPERATURE OF 298 K, AND IT CONTAINED A 5 M**3 SODIUM POOL AT AN INITIAL TEMPERATURE OF 566 K. THE SYSTEM WAS ADIABATIC EXCEPT FOR HEAT TRANSFER BETWEEN THE POOL AND THE ATMOSPHERE. THERE WERE NO CHEMICAL REACTIONS.

7. TEST: CHECK THE POOL-ATMOSPHERE HEAT BALANCE.

8. RESULTS OF TEST: THE INITIAL TEST RUNS IN THIS SERIES SHOWED THAT THE CONTAIN CODING NEEDED CORRECTION. FOR EXAMPLE, IN ONE CASE THE CELL ATMOSPHERE WAS HEATED BY THE SODIUM POOL TO TEMPERATURES HIGHER THAN THAT OF THE POOL. CHECKS OF THE HEAT BALANCE SHOWED THAT THE ATMOSPHERE WAS GAINING FOUR OR FIVE TIMES THE HEAT GIVEN UP BY THE POOL.

   CHECKS OF THE CODING IN CONTAIN REVEALED AN INCONSISTENCY BETWEEN THE POOL AND THE ATMOSPHERE HEAT-BALANCE ROUTINES. TWO CORRECTIONS WERE MADE. ONE MADE THE UNITS CONSISTENT IN THE TWO ROUTINES, THE OTHER CORRECTED AN INITIALIZATION PROBLEM. ONCE THESE CORRECTIONS WERE MADE, THE HEAT GAINED BY THE AIR AGREED VERY CLOSELY WITH THE HEAT LOST FROM THE POOL.

   THE HEATUP OF THE CELL ATMOSPHERE AND THE COOLING TREND OF THE POOL AS PREDICTED BY CONTAIN ARE ILLUSTRATED IN FIGURES PQ-01 AND PQ-02. BOTH CURVES FLATTEN OUT SLIGHTLY WITH TIME. THIS BEHAVIOR IS QUALITATIVELY CORRECT BECAUSE THE HEAT TRANSFER BETWEEN THE POOL AND THE ATMOSPHERE MUST DIMINISH AS THE TEMPERATURE DIFFERENTIAL BETWEEN THEM DIMINISHES WITH TIME.

9. COMMENTS: NONE.

10. SUGGESTIONS FOR ADDITIONAL TESTS: TESTS SHOULD BE CONDUCTED TO CHECK POOL-TO-STRUCTURE AND ATMOSPHERE-TO-STRUCTURE HEAT TRANSFER. CHECKS SHOULD BE MADE OF BOTH THE HEAT BALANCES AND THE HEAT TRANSFER RATES.

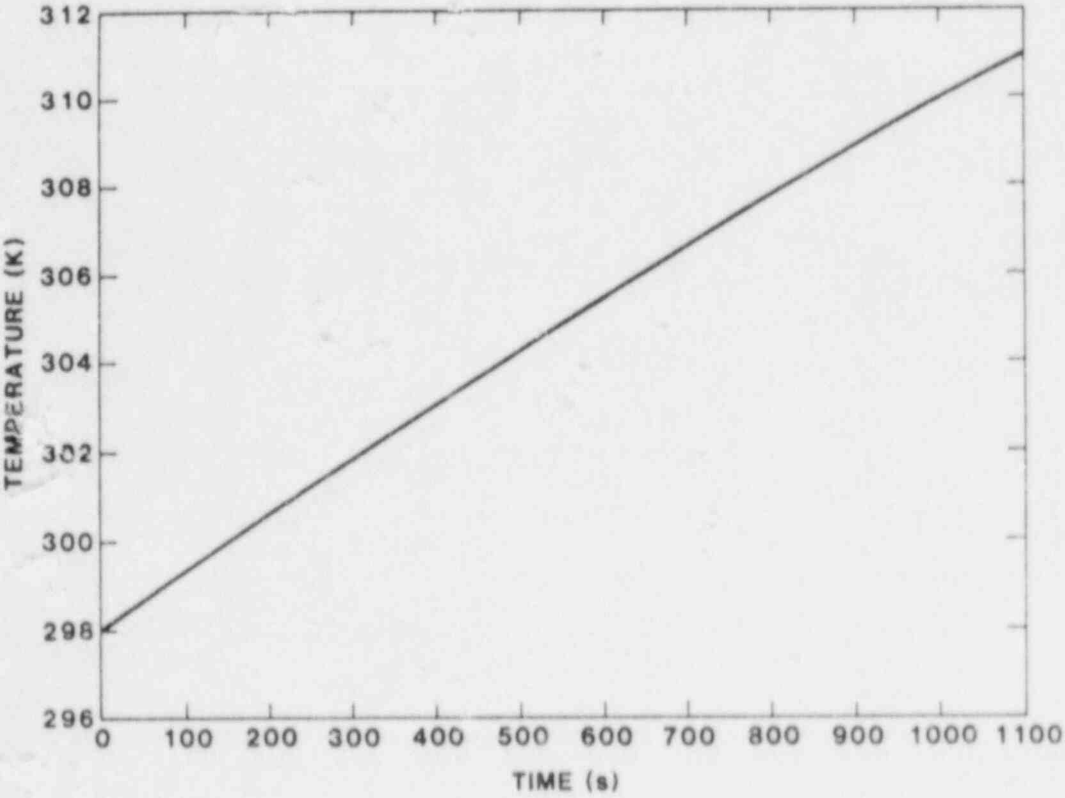

Figure PQ-01 Cell gas temperature during pool-to-atmosphere heat transfer (Test PQ03).

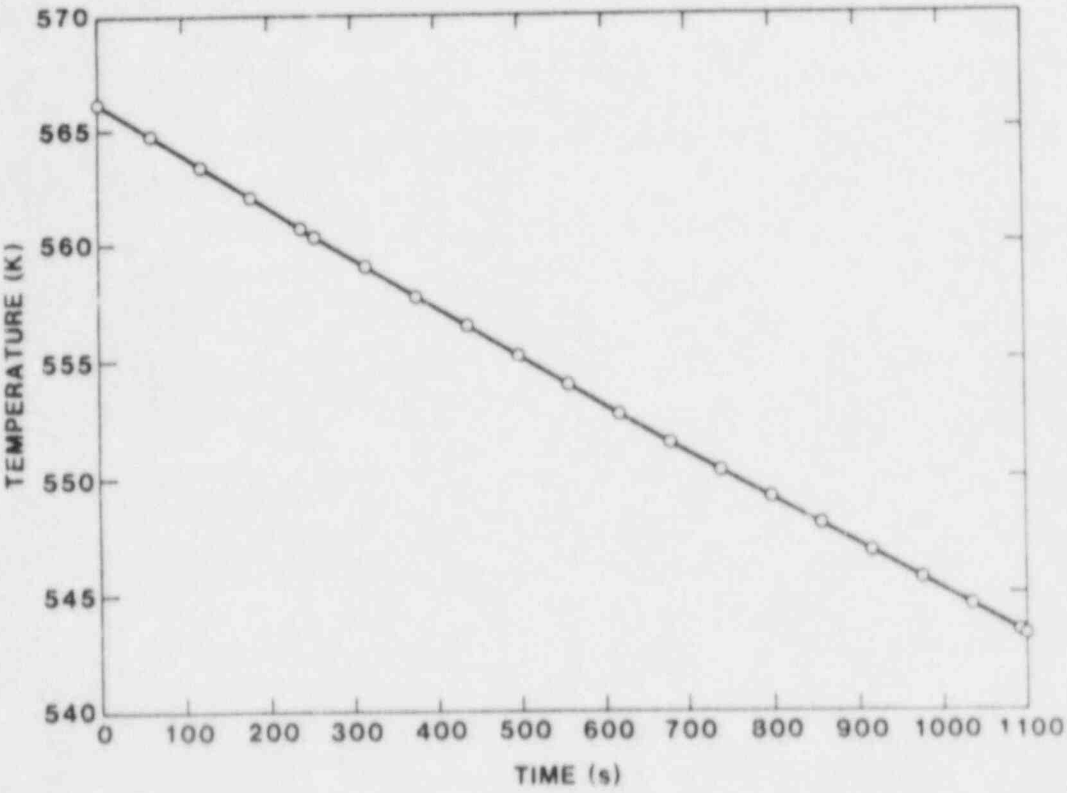

Figure PQ-02 Pool temperature during pool-to-atmosphere heat transfer (Test PQ03).

Suppporting Analysis: PQ Series - Pool-to-Atmosphere Heat Transfer

In this problem, the system consisted of an adiabatic air-filled cell that also contained a pool of sodium. There are no heat sinks or sources, and no chemical reactions occur. The pool is initially hotter than the atmosphere. The check calculations merely compared the heat loss from the pool with the heat gained by the cell atmosphere.

Heat loss from the pool:

$$Q_P = M_{Na}\int_{T_{1_P}}^{T_{2_P}} C_p(T)dT \qquad (3.5\text{-}1)$$

where M_{Na} = mass of sodium in pool

C_p = specific heat of liquid sodium

$C_p(T)$ was used in the form

$$C_p(T) = A + BT + CT^{-2} + DT^2$$

Heat gained by the air:

$$Q_A = M_A Cv(T_{2_A} - T_{1_A})$$

where

M_A = mass of air

C_v = specific heat of air at constant volume (average for range from T_{1_A} to T_{2_A})

The subscript A denotes atmosphere conditions, and the subscript P denotes pool conditions.

3.5.2 Series PB - Pool Heatup and Boiling

The PB test series was conducted to check primarily the modeling of the pool thermodynamics. Checks were also made of the atmosphere thermodynamics when vapor from the pool entered the atmosphere. In each of the tests a fission-product source was used to heat a liquid pool. Tests were made with both sodium and water pools. The parameters that were checked included pool heatup rate (time to reach boiling), boiling rate, and time for the pool to boil dry. For some tests the atmosphere temperature and pressure were checked once boiling had commenced. Qualitative checks were also made of the CONTAIN feature that provides for the addition of condensate to a pool.

The initial tests in this series indicated that CONTAIN's pool models were giving erroneous results. The time for the pool to reach its boiling point compared well with the predictions obtained by hand calculations. However, the pool boiling rate (rate of vapor generation) was much too high, and the pool temperature rose substantially above the boiling point once boiling began. In addition, these tests indicated that condensate was not being added to a pool when this was supposed to happen.

An examination of the coding revealed several errors. These errors were corrected using appropriate updates. Tests PB05 and PB06 were performed after making these corrections. Results of these two tests agreed very closely with predictions from hand analyses. The one exception was the addition of condensate to a pool. This aspect was not corrected.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: PB01, PB02, AND PB03 USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL2, TL3, TL4A
3. TITLE OF TEST: SODIUM-POOL HEATUP AND BOILING
4. CODE VERSION (DATE): 324 (5-7,10,12-82)
5. ACTIVE MODULES OR OPTIONS: POOL THERMODYNAMICS (SINTER), FISSION-PRODUCT HEATING, ATMOSPHERE THERMODYNAMICS, INTERCELL FLOW, AND ATMOSPHERE-TO-STRUCTURE HEAT TRANSFER
6. CONTAINMENT CONFIGURATION AND SOURCES: TWO INTERCONNECTED CELLS. CELL #1 CONTAINS A SODIUM POOL AT AN INITIAL TEMPERATURE OF 400 K AND OCCUPYING A VOLUME OF 500 M**3. THIS POOL CONTAINS A LARGE FISSION-PRODUCT HEAT SOURCE THAT REMAINS CONSTANT WITH TIME. CELL #1 HAS A TOTAL VOLUME OF 1000 M**3 AND HAS A NITROGEN ATMOSPHERE. IT CONNECTS TO CELL #2, WHICH ALSO HAS A NITROGEN ATMOSPHERE AND A TOTAL VOLUME OF 10000 M**3. BOTH CELLS ARE INITIALLY AT 400 K. FOR TESTS PB01 AND PB03 THE CELLS CONTAINED NO HEAT SINKS OR SOURCES OTHER THAN THE FISSION PRODUCTS. TEST PB02 INCLUDED A SHALLOW SODIUM POOL IN CELL #2 AND A LARGE STRUCTURE ACTING AS A VAPOR-CONDENSATION SURFACE.

7. TEST: HAND CALCULATIONS WERE MADE TO PREDICT THE TIME AT WHICH THE POOL IN CELL #1 WOULD REACH THE BOILING POINT AND THE VAPORIZATION RATE ONCE BOILING BEGAN. CONSISTENCY CHECKS WERE MADE OF THE CONTAIN-PREDICTED ATMOSPHERE TEMPERATURES AND PRESSURES AT SPECIFIC TIMES. FOR TEST PB02, SEMIQUANTITATIVE TESTS WERE MADE TO DETERMINE WHETHER CONTAIN WAS PROPERLY HANDLING THE ADDITION OF CONDENSATE TO THE POOL IN CELL #2. THE HAND-CALCULATED RESULTS WERE COMPARED WITH THOSE FROM CONTAIN.

8. RESULTS OF TEST: TEST PB02 PROVED TO BE THE MOST INFORMATIVE, AND THE FOLLOWING RESULTS ARE DERIVED PRIMARILY FROM THIS TEST:

* TIME TO POOL BOILING:

HAND CALCULATION	5443 S
CONTAIN	5430 S

THE CONTAIN RESULT COMPARES VERY FAVORABLY WITH THE PREDICTION FROM THE HAND CALCULATION. THIS AGREEMENT WAS ACHIEVED WHEN THE "DENSITY=CONSTANT" OPTION WAS USED. THIS OPTION HOLDS THE POOL DENSITY CONSTANT WITH CHANGES IN TEMPERATURE. WHEN THE CODE IS ALLOWED TO ADJUST THE POOL DENSITY BECAUSE OF TEMPERATURE CHANGES, THE MASS ASSOCIATED WITH ANY EXPANSION BEYOND THE INITIAL POOL VOLUME IS APPARENTLY LOST. THIS EFFECTIVELY REDUCES THE MASS BEING HEATED; CONSEQUENTLY, IT HEATS UP AT A FASTER RATE, AND THE CODE GIVES ERRONEOUS RESULTS FOR THIS CASE (BOILING AT ~4185 S VS 5430 S).

TIME AND BOILING RATE:	TIME, S	RATE, KG/S
HAND CALCULATIONS		20.93
CONTAIN	~5610	277.37
	~5720	469.84
	~5830	612.98
	~5940	690.28
	~6050	692.20

THE BOILING RATES PREDICTED BY CONTAIN CONTINUE TO INCREASE WITH TIME TO VERY HIGH AND UNREALISTIC VALUES. EVEN AT THE EARLY BOILING TIMES THE RATES ARE MORE THAN A FACTOR OF 10 HIGHER THAN THEY SHOULD BE. THE PRESENT CODING ASSUMES THAT THE BOILING POINT IS FIXED AND IS INDEPENDENT OF PRESSURE. THEREFORE, THE BOILING RATE SHOULD REMAIN CONSTANT AS LONG AS THE POOL HEATING IS CONSTANT. THE BOILING RATES PREDICTED BY CONTAIN ARE OBVIOUSLY IN CONSIDERABLE ERROR.

* POOL TEMPERATURES:

BECAUSE THE BOILING POINT USED IN CONTAIN IS INDEPENDENT OF SYSTEM PRESSURE, THE POOL TEMPERATURE SHOULD REMAIN CONSTANT AT THE BOILING POINT ONCE THIS TEMPERATURE IS REACHED. THE CONTAIN RESULTS SHOW THE POOL TEMPERATURE CLIMBING FROM THE 1154 K BOILING POINT AT 5430 S TO 1283 K AT 6050 S WHEN THE CALCULATION OF POOL CONDITIONS WAS TERMINATED.

* ATMOSPHERE TEMPERATURES AND PRESSURES:

FOR THIS CHECK THE CONTAIN VALUES FOR CELL ATMOSPHERE TEMPERATURE AND MOLAR CONSTITUENTS WERE USED TO CALCULATE THE CELL PRESSURE. THESE HAND CALCULATIONS WERE THEN COMPARED WITH THE PRESSURE PREDICTED BY CONTAIN. THE HAND CALCULATION USED THE VAPOR PRESSURE OF SODIUM AT

THE INDICATED TEMPERATURE PLUS THE PARTIAL PRESSURE OF NITROGEN TO ARRIVE AT THE TOTAL PRESSURE. THE COMPARISON AT TIME = 5500 S IS AS FOLLOWS:

HAND CALCULATION	1.5992E6 PA
CONTAIN	0.1380E6 PA

HERE, AGAIN, THERE ARE PROBLEMS WITH THE WAY THE CODE IS HANDLING ATMOSPHERE THERMODYNAMICS WHEN SODIUM VAPOR IS PRESENT. (CAUSE OF THIS PROBLEM RESOLVED AND CORRECTED WITH SUBSEQUENT UPDATE)

ANOTHER PROBLEM WITH THE ATMOSPHERE THERMODYNAMICS IS THAT THE ATMOSPHERE TEMPERATURES AS PREDICTED BY CONTAIN RISE VERY RAPIDLY ONCE BOILING BEGINS AND RAPIDLY EXCEED THE SODIUM-VAPOR TEMPERATURE BASED ON THE POOL CONDITIONS. AT THE 6000-S POINT IN THE CALCULATION THE CELL #1 ATMOSPHERE TEMPERATURE WAS 3112 K. ALTHOUGH NO HAND CALCULATIONS OF THE CELL ATMOSPHERE CONDITIONS HAVE BEEN MADE, THE CONTAIN RESULTS APPEAR TO BE WRONG.

* ADDITION OF CONDENSED SODIUM TO SECOND POOL:
THE CODING IN CONTAIN IS INTENDED TO ALLOW FOR THE ADDITION OF CONDENSATE FROM VERTICAL SURFACES TO EXISTING POOLS. TEST PB02 INCLUDED A CONDENSING STRUCTURE AND A SHALLOW POOL TO TEST THIS FEATURE. THE CONTAIN RESULTS INDICATE THAT CONDENSATION IS OCCURRING, BUT THE CONDENSATE IS NOT BEING ADDED TO THE POOL. THE CONDENSATE APPEARS TO BE LOST FROM THE SYSTEM.

9. <u>COMMENTS</u>: THE POOL THERMODYNAMICS IN CONTAIN CURRENTLY PERFORMS RATHER POORLY. THE POOL HEATUP TO BOILING IS ACCURATELY PREDICTED AS LONG AS THE "DENSITY = CONSTANT" OPTION IS USED, BUT SUBSEQUENT TO BOILING, PREDICTED CONDITIONS APPEAR TO BE IN CONSIDERABLE ERROR. THE BOILING RATES ARE TOO HIGH, THE POOL TEMPERATURE DOES NOT REMAIN CONSTANT AS IT SHOULD, AND THE PREDICTED ATMOSPHERE TEMPERATURE/PRESSURE COMBINATION IS IN ERROR. IN ADDITION, CONDENSATE IS NOT ADDED TO AN INITIAL POOL AS IS INTENDED IN THE CODE. THIS PORTION OF CONTAIN APPEARS TO BE IN NEED OF SIGNIFICANT REVISION AND CORRECTION.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

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1. PROBLEM: ID NO. PB01-01 2. LEVEL: PL3 3. RESOLVED? PARTIALLY (SEE TESTS PB05 AND PB06)
4. DESCRIPTION: CODE RESULTS ARE IN ERROR WITH RESPECT TO: (1) POOL HEATUP AND BOILING, (2) ATMOSPHERE CONDITIONS WHEN SODIUM VAPOR IS PRESENT, AND (3) THE ADDITION OF SODIUM CONDENSATE TO AN EXISTING POOL.
5. DATE PROBLEM RESOLVED: ~8-82; (1) and (2) RESOLVED.

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CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: PB04 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A

3. TITLE OF TEST: WATER-POOL HEATUP AND BOILING

4. CODE VERSION (DATE): 312 (5-12-82)

5. ACTIVE MODULES OR OPTIONS: POOL THERMODYNAMICS (SINTER), FISSION-PRODUCT HEATING, ATMOSPHERE THERMODYNAMICS, INTERCELL FLOW, AND ATMOSPHERE-TO-STRUCTURE HEAT TRANSFER

6. CONTAINMENT CONFIGURATION AND SOURCES: TWO INTERCONNECTED CELLS. CELL #1 CONTAINS A WATER POOL AT AN INITIAL TEMPERATURE OF 300 K AND OCCUPYING A VOLUME OF 500 M**3. THIS POOL CONTAINS A LARGE FISSION-PRODUCT HEAT SOURCE THAT REMAINS CONSTANT WITH TIME. CELL #1 HAS A TOTAL VOLUME OF 1000 M**3 AND A NITROGEN ATMOSPHERE. IT CONNECTS TO CELL #2 WHICH ALSO HAS A NITROGEN ATMOSPHERE AND A TOTAL VOLUME OF 10000 M**3. BOTH CELLS ARE INITIALLY AT 300 K. NO HEAT SINKS OR SOURCES OTHER THAN THE FISSION PRODUCTS ARE PRESENT.

7. TEST: HAND CALCULATIONS WERE MADE TO PREDICT THE TIME AT WHICH THE POOL IN CELL #1 WOULD REACH THE BOILING POINT AND THE VAPORIZATION RATE ONCE BOILING BEGAN. THE ATMOSPHERE PRESSURE WAS CALCULATED FOR THE TEMPERATURE AND MOLE FRACTIONS GIVEN BY CONTAIN. THESE HAND-CALCULATED RESULTS WERE COMPARED WITH THE RESULTS GIVEN BY CONTAIN.

8. RESULTS OF TEST:

* TIME TO POOL BOILING:

HAND CALCULATIONS	1867 S
CONTAIN	1890 S

THE AGREEMENT HERE IS QUITE REASONABLE. THESE RESULTS WERE ACHIEVED USING THE "DENSITY=CONSTANT" OPTION PROVIDED IN CONTAIN. ALTHOUGH NOT SPECIFICALLY TESTED FOR THE WATER POOL, IT IS SUSPECTED THAT WITHOUT THIS OPTION THE PREDICTED TIME TO BOILING WOULD BE IN ERROR AS IT WAS FOR THE SODIUM-POOL (BOILING) TEST (SEE PB01).

* BOILING RATE: FOR THE CONSTANT HEAT SOURCE EMPLOYED IN THIS TEST THE BOILING RATE SHOULD HAVE BEEN 36.39 KG/S. AT THIS RATE THE POOL DEPTH SHOULD HAVE DROPPED FROM 10 M TO 9.67 M IN THE INTERVAL BETWEEN 1890 S AND 2340 S. THE CONTAIN RESULTS GAVE A POOL DEPTH OF 3.91 M AT 2340 S. THUS CONTAIN IS CALCULATING MUCH TOO HIGH A BOILING RATE (BY A FACTOR OF ABOUT 20).

* POOL TEMPERATURES: AS IN THE SODIUM-POOL TESTS, THE WATER POOL DID NOT MAINTAIN A CONSTANT TEMPERATURE DURING BOILING. THE TEMPERATURE CLIMBED FROM 373 K TO OVER 400 K AT THE TERMINATION OF THE CALCULATION.

* ATMOSPHERE TEMPERATURES AND PRESSURES: CONTAIN MOLAR FRACTIONS AND ATMOSPHERE TEMPERATURES AT SELECTED TIMES WERE USED TO CALCULATE THE CORRESPONDING PRESSURE.

CELL #	TIME, S	CELL PRESSURE, PA	
		CALCULATED	CONTAIN
1	1980	1.254E5	1.240E5
2	2220	1.520E5	1.511E5

THESE RESULTS SHOW FAIRLY GOOD AGREEMENT BETWEEN THE CONTAIN CELL PRESSURES AND THOSE BASED ON HAND CALCULATIONS.

9. COMMENTS: THE CONTAIN RESULTS FOR WATER-POOL HEATUP-TO-BOILING AND FOR THE ATMOSPHERE TEMPERATURES AND PRESSURES WITH WATER VAPOR PRESENT AGREE QUITE CLOSELY WITH THE PREDICTIONS FROM HAND CALCULATIONS. HOWEVER, THE BOILING RATE AND POOL TEMPERATURES ONCE BOILING HAS STARTED APPEAR TO BE IN CONSIDERABLE ERROR.

10. SUGGESTIONS FOR ADDITIONAL TESTS: TEST THE ADDITION OF WATER CONDENSATE TO AN EXISTING WATER POOL.

==

1. PROBLEM: ID NO. PB04-01 2. LEVEL: PL03 3. RESOLVED? NO
4. DESCRIPTION: THE VAPORIZATION RATE FROM A BOILING WATER POOL IS SIGNIFICANTLY IN ERROR. ALSO, BOILING-POOL TEMPERATURES INCREASE WITH TIME RATHER THAN REMAIN CONSTANT AS WAS INTENDED IN THE CODING.
5. DATE PROBLEM RESOLVED:

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CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: PB05(ST) AND PB06 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A

3. TITLE OF TEST: SODIUM-POOL HEATUP AND BOILING

4. CODE VERSION (DATE): 324 (8-5-82) USED UPDATES "KKMMOD", "MODBOIL", AND "MODTRI"

5. ACTIVE MODULES OR OPTIONS: POOL THERMODYNAMICS (SINTER), FISSION-PRODUCT HEATING, ATMOSPHERE THERMODYNAMICS

6. CONTAINMENT CONFIGURATION AND SOURCES: TEST PB05 USED A SINGLE CELL WITH A SODIUM POOL AT AN INITIAL TEMPERATURE OF 1050 K AND OCCUPYING A VOLUME OF 500 M**3. THIS POOL CONTAINED A LARGE FISSION-PRODUCT HEAT SOURCE THAT REMAINED CONSTANT WITH TIME. THIS CELL HAD A TOTAL VOLUME OF 1.0E5 M**3 AND A NITROGEN ATMOSPHERE. TEST PB06 WAS SIMILAR TO PB05 EXCEPT ITS POOL VOLUME WAS 50 RATHER THAN 500 M**3, AND THE FISSION-PRODUCT HEAT SOURCE WAS ALSO SCALED DOWN BY A FACTOR OF 10. NO OTHER HEAT SINKS OR SOURCES WERE USED IN EITHER TEST. THE SYSTEMS WERE ADIABATIC.

7. TEST: HAND CALCULATIONS WERE MADE TO PREDICT THE TIME AT WHICH THE POOL WOULD BEGIN TO BOIL, THE BOILING RATE, AND THE TIME AT WHICH THE POOL WOULD BOIL DRY. CHECKS WERE MADE OF THE ATMOSPHERE TEMPERATURE AND PRESSURE AT THE TIME OF BOILDRY FOR TEST PB06. ATMOSPHERE PRESSURE AND TEMPERATURE CHECKS WERE MADE AT 1000 S FOR PB05.

8. RESULTS OF TEST:

* TIME TO POOL BOILING:	PB05	PB06
HAND CALCULATIONS	618 S	617 S
CONTAIN	620 S	620 S

THE CONTAIN RESULTS COMPARE VERY FAVORABLY WITH THE PREDICTIONS FROM THE HAND CALCULATIONS. THIS AGREEMENT WAS ACHIEVED WHEN THE "DENSITY=CONSTANT" OPTION WAS USED.

* BOILING RATE:	PB05	PB06
HAND CALCULATIONS	20.93 KG/S	2.093 KG/S
CONTAIN	20.89	2.083

THESE RESULTS SHOW THAT THE UPDATES USED GIVE GOOD AGREEMENT BETWEEN CONTAIN AND THE HAND CALCULATIONS.

* POOL TEMPERATURES:
THE POOL TEMPERATURES IN THE CONTAIN RUNS REMAIN CONSTANT IN TIME AT 1154 K ONCE BOILING BEGINS. THIS IS AS IT SHOULD BE.

* ATMOSPHERE TEMPERATURES AND PRESSURES:
THE ATMOSPHERE CONDITIONS FOR TEST PB05 WERE CHECKED AT 1000 S INTO THE PROBLEM. FOR TEST PB06 THE CONDITIONS WERE CHECKED AT BOILDRY.

FOR TEST PB05:	TEMP, K	PRESS, PA
CALCULATED	884.4	2.251E5
CALCULATED(ALT. DATA SOURCE)	898.4	
CONTAIN	861.3	2.181E5
FOR TEST PB06:		
CALCULATED	1157	3.927E5
CONTAIN	1169	4.080E5

THESE RESULTS, AGAIN, SHOW FAIRLY GOOD AGREEMENT BETWEEN CONTAIN AND THE HAND ANALYSIS. AS SHOWN ABOVE, USE OF DATA FROM DIFFERENT SOURCES CAN ALSO LEAD TO DIFFERENCES IN THE PREDICTED CONDITIONS.

* TIME TO BOILDRY:
TEST PB06 WAS THE ONLY ONE CONTINUED THRU BOILDRY OF THE POOL.

CALCULATED TIME TO BOILDRY	18882 S
CONTAIN " " "	18968 S

THE AGREEMENT HERE IS ALSO QUITE GOOD. THE DIFFERENCE CAN BE ACCOUNTED FOR BY THE DIFFERENCE IN THE DATA SOURCES USED.

FIGURES PB-01, -02, AND -03 DISPLAY SOME OF THE RESULTS OBTAINED IN TEST PB05. FIGURE PB-01 SHOWS THE CELL ATMOSPHERE TEMPERATURE VS TIME. BECAUSE HEAT TRANSFER BETWEEN THE POOL AND THE GAS WAS TURNED OFF IN THIS TEST, THE CELL'S GAS TEMPERATURE DOES NOT CHANGE UNTIL SODIUM VAPOR ENTERS THE ATMOSPHERE. THE POOL BEGINS TO BOIL AT ABOUT 620 S INTO THE PROBLEM. FIGURE PB-02 SHOWS THE INCREASE IN SODIUM-VAPOR CONTENT IN THE ATMOSPHERE WITH TIME. THE BOILING RATE WAS QUITE HIGH FOR THIS TEST. FIGURE PB-03 GIVES THE POOL TEMPERATURE AS A FUNCTION OF TIME. THE PLOT SHOWS THAT THE POOL HEATUP RATE IS CONSTANT. THIS IS AS IT SHOULD BE SINCE THE POOL HEAT SOURCE REMAINED CONSTANT. THE PLOT ALSO SHOWS THAT THE POOL TEMPERATURE REMAINS STEADY AT THE BOILING POINT OF SODIUM (1154 K) ONCE THE BOILING POINT IS REACHED.

9. COMMENTS: THE TREATMENT OF THE POOL THERMODYNAMICS IN CONTAIN HAS BEEN SUBSTANTIALLY CORRECTED SINCE THE RESULTS REPORTED IN TEST REPORT PB01 WERE OBTAINED. SEVERAL UPDATES WERE EMPLOYED TO ACHIEVE THE IMPROVEMENTS IN THE CODE RESULTS AS NOTED HERE. THESE UPDATES WILL BE INCORPORATED IN LATER VERSIONS OF THE CODE. NOTE THAT CURRENT VERSIONS OF CONTAIN ASSUME A FIXED BOILING POINT FOR THE COOLANT. THIS SIMPLIFIED APPROACH CAN LEAD TO SIGNIFICANT ERRORS IN THE CODE'S PREDICTIONS. A MORE REALISTIC TREATMENT IS NEEDED.

   FOR TEST PROBLEM PB06 THE CALCULATIONS WERE CARRIED THROUGH TO THE POINT OF POOL BOILDRY. AT THIS POINT THE CODE ABORTED THE RUN, BECAUSE THE CODE WILL NOT RUN BEYOND THIS POINT FOR THE CONDITIONS SET UP IN THIS PROBLEM.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

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1. PROBLEM: ID NO. PB05-01   2. LEVEL: PL03   3. RESOLVED: NO
4. DESCRIPTION: THE CODE ASSUMES A FIXED BOILING POINT FOR THE COOLANT. THIS CAN LEAD TO UNREALISTIC OR ERRONEOUS RESULTS FOR MANY PROBLEMS. A MORE REALISTIC BOILING MODEL IS NEEDED.
5. DATE PROBLEM RESOLVED:

==

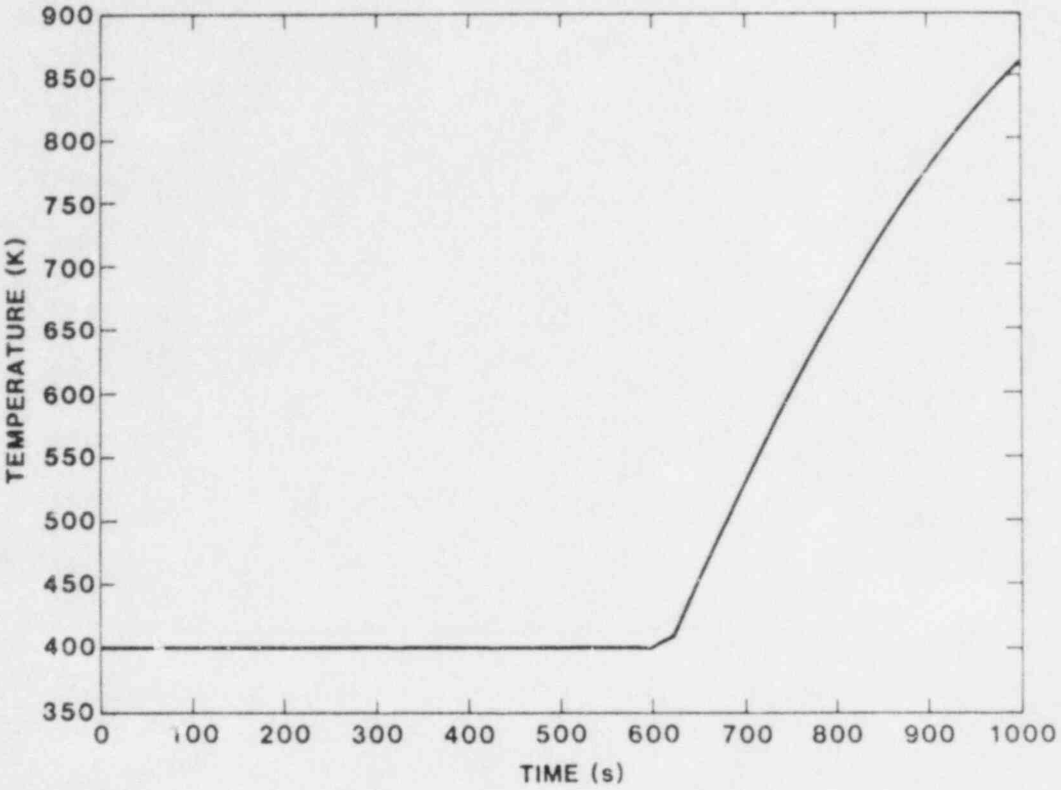

Figure PB-01 Cell gas temperature during pool-boiling test (Test PB05).

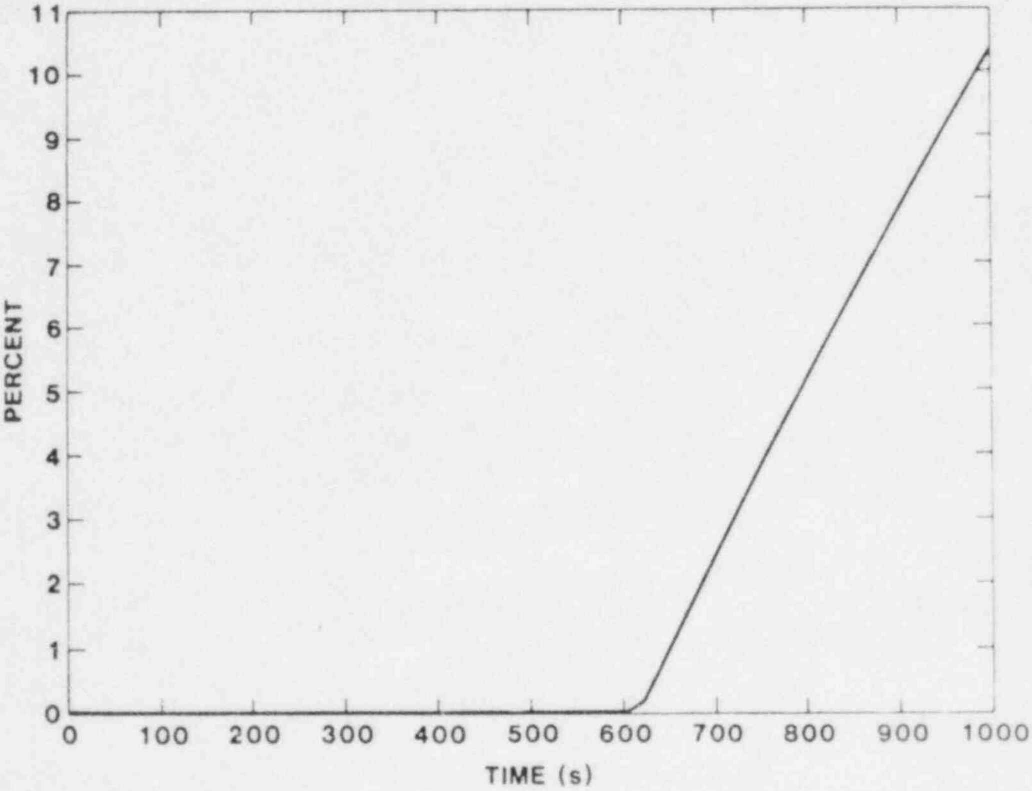

Figure PB-02 Concentration of sodium vapor in atmosphere during pool-boiling test (Test PB05).

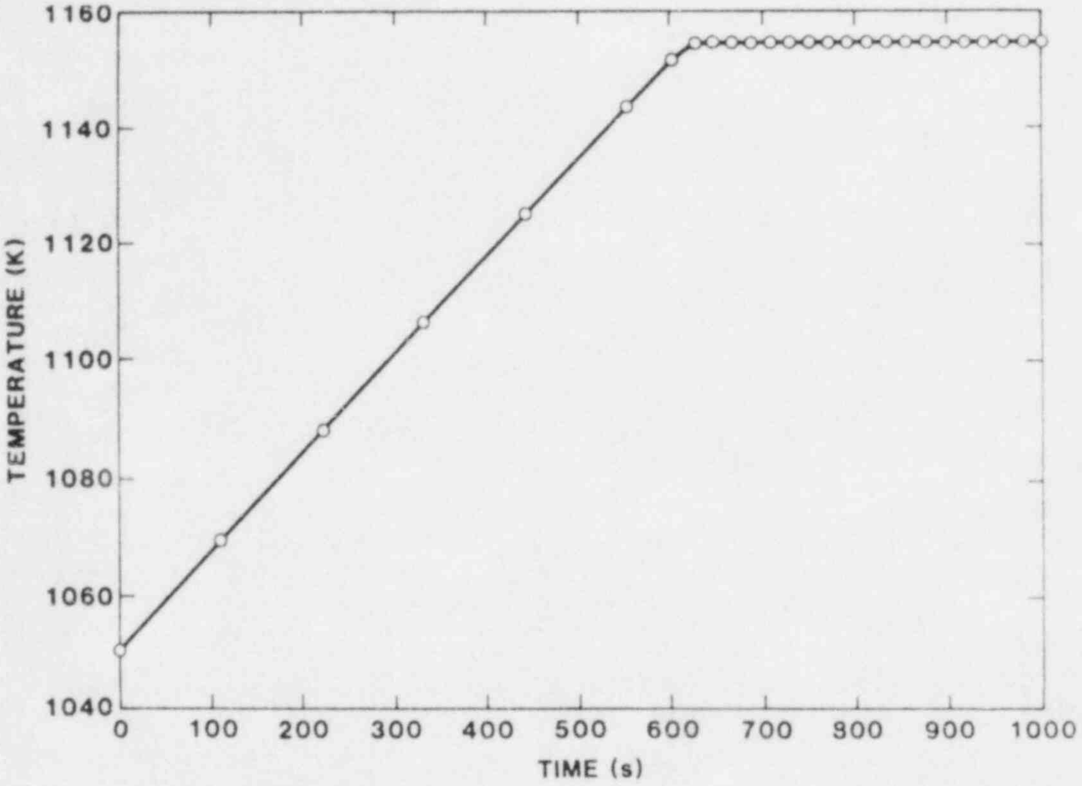

Figure PB-03 Pool temperature during pool-boiling test (Test PB05).

Supporting Analysis: PB Series - Pool Heatup and Boiling

Consider a sodium or water pool located in a nitrogen-filled cell. The liquid pool has a constant heat source. There are no other energy sinks or sources. The pool is adiabatic except for heat lost to the atmosphere via vapor transport once boiling begins. The initial pool temperature is below the boiling point. For this situation, calculate the time at which the pool will reach its boiling point, the boiling rate (vapor-generation rate), and the time at which all liquid will be boiled away (boildry time). Also, predict the atmosphere conditions once boiling begins.

A. Time to Boiling:

The energy required to bring the pool to its boiling point is

$$Q_B = m_i \int_{T_i}^{T_B} C_p(T)dT \qquad (3.5\text{-}3)$$

where

m_i = initial mass of liquid in the pool

T_i = initial temperature of the pool

T_B = temperature at boiling point

C_p = specific heat of the liquid

With a steady heat source, the time to boil is given by:

$$t_B = \frac{Q_B}{\dot{Q}} = \frac{m_i \int_{T_i}^{T_B} C_p(T)dt}{\dot{Q}} \qquad (3.5\text{-}4)$$

where

$\dot{Q}$ = rate of heat input to pool

B. Boiling Rate:

Once boiling begins, the boiling rate is determined by the heat input rate and the heat of vaporization,

$$\dot{m}_B = \frac{\dot{Q}}{h_{fg}} \qquad (3.5\text{-}4)$$

where

$h_{fg} = h_g - h_f$ = heat of vaporization of the liquid

C. Boildry Time:

The time at which boildry should occur is

$$t_D = t_B + \frac{m_i h_{fg}}{\dot{Q}} = t_B + \frac{m_i}{\dot{m}_B} \qquad (3.5\text{-}5)$$

D. Atmosphere Conditions:

For the case where the cell atmosphere is cooler than the pool at its boiling point, the atmosphere will rapidly become saturated with vapor once pool boiling begins. The energy balance at any time after the onset of boiling is

$$m_T h_{g,i} = m_A(h - RT)_{A,2} + (1 - X)m_T h_{f,2} + Xm_T(h - pv)_{g,2} - m_A(h - RT)_{A,1} \qquad (3.5\text{-}6)$$

where

m_T = total mass of condensible vapor that has entered the atmosphere by the specified time

$h_{g,i}$ = enthalpy of the vapor entering the atmosphere

m_A = mass of noncondensible gas in the atmosphere

X = vapor quality

and the subscripts have the following meanings:

f = liquid
g = vapor
A = atmosphere gas
i = condition of vapor entering atmosphere
1 = initial atmosphere conditions
2 = end-state conditions (at selected times)

Note that

$$X = \frac{m_g}{m_T} \text{ and } v_g = \frac{V}{m_g} \qquad (3.5\text{-}7)$$

where

V = total cell volume
v_g = specific volume of vapor
m_g = mass of vapor

Hence

$$X = \frac{V}{v_g m_T} \qquad (3.5\text{-}8)$$

Separating knowns and unknowns

$$m_T h_{g,1} + m_A (h - RT)_{A,1} = m_A (h - RT)_{A,2} + (1 - X) m_T h_{f,2} + X m_T (h - pv)_{g,2} \quad (3.5\text{-}9)$$

The solution is found by iterating on the final temperature, T_2, and by using the corresponding properties at that final temperature.

The final system pressure is calculated from the following equation:

$$P_2 = P_{sat(g,2)} + \frac{m_A R T_2}{V} \quad (3.5\text{-}10)$$

SERIES PB STANDARD TEST INPUT DATA SET

```
&&      ------------------ PB05(ST) ----------------------------------------

CONTROL=9 1 3 2 2 1 20 0 1 0
MATERIAL
COMPOUND N2 O2 H2 HE NAV NAL   FE
FISSION
DUM1 DUM2
TIMES 100.0 0.0 10.0 100.0 600.0 1.0 20.0 1000.0 1.0
FLOWS
PRFISS PRFLOW PRPOOL
PROPERTY NAV 0 0 0 0 0 BS -1 0 EOI
FISSION
1  NAL
2
DUM1 DUM2
1.0E12 1.0E15
8.2091E7 1.0
FPM-CELL=1
HOST=NAL 1.0 0.0
EOI
TITLE
        TEST OF POOL HEATUP AND BOILING   * DENSITY=CONSTANT  USED *
 CASE PB05(ST):  500 M**3 SODIUM POOL WITH LARGE FISSION PRODUCT HEAT SOURCE
         NO HEAT SINKS OR STRUCTURES.  SINGLE CELL SYSTEM. GAS BAGGED.
FAST
CELL=1
CONTROL=17 3 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
TITLE
    CELL #1 WITH LARGE SODIUM POOL
GEOMETRY
100000.0 15.0
ATMOS=1
1.0001E5 400.0
N2 1.0
POOL
0 0 0 1 50.0
3 10.0
1050.0
1050.0 1050.0 0.1 1050.0 1
NAL 1.0
DENSITY=CONSTANT
EOI
HT-TRAN OFF OFF OFF OFF OFF OFF OFF
EOF
```

3.5.3 Series PS - Pool Sources

This test series investigated the thermodynamic behavior of pools when source materials were introduced into or removed from them. The different tests employed different source materials, both positive and negative sources, and sources whose temperatures were either higher or lower than the initial pool temperature.

The results of these investigations indicate that materials can indeed be introduced into or removed from pools, but that the subsequent pool heatup or cooldown due to these sources is suspect. Results of tests conducted using source materials with constant specific heats (as coded in CONTAIN) were generally in good agreement with the results of hand analyses. When source materials having variable specific heats were used, the agreement was much poorer. Thus the CONTAIN results appear to be questionable when the pool-sources option is exercised, and this option should be used cautiously.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: PS01 - PS11 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A

3. TITLE OF TEST: POOL SOURCES

4. CODE VERSION (DATE): A20 (11-19 THRU 12-7-82)

5. ACTIVE MODULES OR OPTIONS: POOL THERMODYNAMICS AND SOURCE ROUTINES, ATMOSPHERE THERMODYNAMICS

6. CONTAINMENT CONFIGURATION AND SOURCES: A SINGLE CELL CONTAINING A SODIUM POOL AND A NITROGEN ATMOSPHERE WAS USED. THE INITIAL VOLUME OF POOL MATERIALS RANGED FROM 100 M**3 TO 500 M**3. INITIAL POOL TEMPERATURES OF 1000 K AND 1050 K WERE USED. DIFFERENT MATERIALS WERE INTRODUCED INTO THE POOL AT DIFFERENT RATES AND AT DIFFERENT TEMPERATURES. THE INITIAL CONDITIONS FOR THE VARIOUS TESTS WERE AS FOLLOWS:

	POOL INITIAL CONDITIONS		SOURCE(S)		
TEST	VOLUME, M**3	TEMP, K	MATERIAL	RATE, KG/S	TEMP, K
PS01	500	1050	FE	5	800
PS02	500	1050	FE	5	800
			NA	(-)3	1050
PS03	500	1050	NA	(-)5	600
PS04	100	1050	FE	5	1300
PS05	500	1050	FE	5	1300
PS06	500	1000	NAOH	5	1450
PS07	500	1000	NAOH	5	700
PS08	500	1000	AL2O3	5	1450
PS09	500	1000	AL2O3	5	700
PS10	300	1000	NA2SIO3	5	1350
PS11	300	1000	NA2SIO3	5	650

THE INITIAL TEMPERATURES OF THE SOURCE MATERIALS WERE CHOSEN TO TEST BOTH HEATUP AND COOLDOWN OF THE POOL. IN ADDITION, CONSTANT SPECIFIC HEATS WERE USED FOR SOME MATERIALS AND FOR OTHERS THE SPECIFIC HEATS WERE TREATED BY CONTAIN AS FUNCTIONS OF TEMPERATURE.

7. TEST: HAND CALCULATIONS WERE MADE TO PREDICT POOL TEMPERATURES AS A FUNCTION OF TIME FOR THE CASES WHERE THE SOURCE MATERIAL WAS COOLER THAN THE POOL OF SODIUM. FOR THE CASES WHERE THE SOURCE MATERIAL WAS ABOVE THE SODIUM BOILING POINT, THE TIME TO BOILING WAS CALCULATED. FOR TEST PS08, SODIUM BOILING RATES WERE ALSO CALCULATED. THESE HAND CALCULATIONS WERE COMPARED WITH THE CONTAIN RESULTS.

8. RESULTS OF TEST: THE POOL-SOURCE ROUTINES DO WORK, AND NEGATIVE AS WELL AS POSITIVE SOURCES CAN BE USED IN CONTAIN. HOWEVER, THE AGREEMENT BETWEEN THE CONTAIN RESULTS AND THE RESULTS OF HAND ANALYSES FOR HEATUP OR COOLDOWN OF THE POOL IS NOT ALWAYS AS GOOD AS DESIRED. THE FOLLOWING TABULATION GIVES AN INDICATION OF THE RESULTS OBTAINED. SOURCE MATERIALS FOR EACH TEST ARE INDICATED.

TEST	TEST PARAMETER	CALCULATION	CONTAIN
PS01	POOL TEMP AFTER 8000 S	1038 K	1040 K
	POOL TEMP AFTER 30000 S	1011 K	1017 K
	(5 KG/S FE AT 800 K)		
PS02	POOL TEMP AFTER 8000 S	1038 K	1039 K
	POOL TEMP AFTER 30000 S	1002 K	1005 K
	(5 KG/S FE AT 800 K, -3 KG/S NA AT 1050 K)		
PS03	TIME TO REACH BOILING	14350 S	14550 S
	SODIUM REMAINING AT 30000 S	214828 KG	218500 KG
	(-3 KG/S NA AT 600 K)		
PS04	TIME TO REACH BOILING	13784 S	10100 S
	(5 KG/S FE AT 1300 K)		
PS05	TIME TO REACH BOILING	68925 S	48700 S
	(5 KG/S FE AT 1300 K)		
PS06	TIME TO REACH BOILING	46844 S	46700 S
	(5 KG/S NAOH AT 1450 K)		
PS07	POOL TEMP AFTER 30000 S	924 K	924 K
	(5 KG/S NAOH AT 700 K)		
PS08	TIME TO REACH BOILING	41026 S	41000 S
	SODIUM VAPORIZATION RATE	0.474 KG/S	~0.67 KG/S
	(5 KG/S AL2O3 AT 1450 K)		
PS09	POOL TEMP AFTER 30000 SECONDS	925 K	924 K
	POOL TEMP AFTER 60000 SECONDS	880 K	879 K
	(5 KG/S AL2O3 AT 700 K)		

TEST	TEST PARAMETER	CALCULATION	CONTAIN
PS10	TIME TO REACH BOILING (5 KG/S NA2SIO3 AT 1350 K)	24650 S	20500 S
PS11	POOL TEMP AFTER 60000 SECONDS (5 KG/S NA2SIO3 AT 650 K)	859 K	836 K

THE SOURCE MATERIALS WITH CONSTANT SPECIFIC HEATS WERE NAOH AND AL2O3. FE AND NA2SIO3 HAD SPECIFIC HEATS WHICH VARIED WITH TEMPERATURE. THE AGREEMENT BETWEEN THE HAND-ANALYSIS RESULTS AND THE RESULTS FROM CONTAIN WAS MUCH BETTER FOR TESTS IN WHICH CONSTANT SPECIFIC HEATS WERE USED.

9. COMMENTS: THE RESULTS TABULATED ABOVE INDICATE THAT THE POOL SOURCE ROUTINES ARE WORKING, BUT THAT THE RESULTS ACHIEVED ARE SUSPECT. MUCH BETTER AGREEMENT WAS OBTAINED FOR TESTS WITH CONSTANT-SPECIFIC-HEAT MATERIALS THAN FOR THOSE WITH VARIABLE-SPECIFIC-HEAT MATERIALS. WITH CONSTANT-SPECIFIC-HEAT SOURCES, THE DATA (POOL TEMPERATURES VS TIME) FROM CONTAIN WERE IN GOOD AGREEMENT WITH DATA FROM HAND ANALYSES. EVEN FOR THESE CASES, HOWEVER, THE BOILING RATES (HAND CALCULATED VS CONTAIN) DIFFERED BY MORE THAN 40%. FOR THE TESTS USING VARIABLE-SPECIFIC-HEAT MATERIALS, THE AGREEMENT ON COOLDOWN RATES FOR THE POOL WAS WITHIN 15-20%. FOR HEATUP TESTS USING THESE MATERIALS, THE TIMES TO BOILING DIFFERED BY ABOUT 30-40%.

EARLY RESULTS IN THIS TEST SERIES DEMONSTRATED THE NEED TO USE A MORE STRINGENT VOLUME-FRACTION CRITERION FOR POOL SOURCES THAN IS CURRENTLY USED IN THE UNMODIFIED CONTAIN CODING. THIS CRITERION IS USED TO DETERMINE WHICH MATERIALS IN THE POOL SHOULD BE TAKEN INTO ACCOUNT IN THE POOL HEAT BALANCE AND WHICH SHOULD BE IGNORED. THE CURRENT VOLUME-FRACTION LIMIT BELOW WHICH MATERIALS ARE IGNORED IS 1.0E-6. EVEN AT THIS LIMIT, POOR HEAT BALANCES WERE OBTAINED. THE VOLUME FRACTION LIMIT WAS REDUCED TO 1.0E-10 IN ALL OF THE TESTS NOTED ABOVE. THIS IMPROVED THE RESULTS BUT DID NOT SOLVE ALL OF THE PROBLEMS. THE DEFAULT VOLUME-FRACTION CRITERION FOR POOL MATERIALS SHOULD BE MADE MUCH LESS THAN THE CURRENT VALUE OF 1.0E-6.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

1. PROBLEM: ID NO. PS01-01   2. LEVEL: PL3   3. RESOLVED? NO
4. DESCRIPTION: POOL HEAT BALANCES APPEAR TO BE IN ERROR, ESPECIALLY WHEN SOURCE MATERIALS HAVE VARIABLE SPECIFIC HEATS (AS TREATED IN THE CODE)
5. DATE PROBLEM RESOLVED:

Supporting Analysis: PS Series - Pool Source

In these tests various source materials are introduced into a pool. In addition, materials can be removed from the pool by specifying a negative (-) source. The pool is nearly adiabatic; heat can only be transferred into or out of the pool via the source or pool materials. There are no chemical interactions and no other energy sources or sinks.

The energy balance for the pool is as follows:

$$\text{Energy In} - \text{Energy Out} = \text{Change in Stored Energy} = \text{Final Energy} - \text{Initial Energy}$$

Consider the case where only one source material is introduced into the pool. Then

$$\text{Energy In} = (\dot{m}\ t\ C_p\ T_i)_{si} \tag{3.5-11}$$

where

$\dot{m}$ = mass flow rate

C_p = specific heat

T = temperature

When the material that constitutes the initial pool is the only material removed (negative source),

$$\text{Energy Out} = (\dot{m}\ t\ C_p\ T_o)_p \tag{3.5-12}$$

Under these conditions

$$\text{Final Energy} = [(m - \dot{m}\ t)\ C_p\ T_f]_p + (\dot{m}\ t\ C_p\ T_f)_{si} \tag{3.5-13}$$

and

$$\text{Initial Energy} = (m\ C_p\ T_i)_p \tag{3.5-14}$$

where m is the initial mass of the pool material and the subscripts have the following meanings:

si = material introduced into the pool

p = pool material

i = initial condition of pool or source material (Note: $(T_i)_p$ and $(T_i)_{si}$ are not necessarily equal)

f = end-state condition of pool materials

o = end-state condition of material removed from the pool

Hence

$$(\dot{m}tC_pT_i)_{si} - (\dot{m}tC_pT_o)_p = [(m - \dot{m}\,t)C_pT_f]_p + (\dot{m}tC_pT_f)_{si} - (mC_pT_i)_p \qquad (3.5\text{-}15)$$

If the specific heats of the materials involved are relatively constant over the temperature range involved, T_f can be solved for directly as a function of time t. If the specific heats vary significantly with temperature, they can be expressed as functions of temperature. The resulting expression can be solved for $T_f(t)$, or an iterative trial and error solution may be used.

3.5.4 Series PC - Pool Chemistry

CONTAIN allows user-specified chemical reactions to occur in pools. This test series exercised this option and checked the accuracy of the code results. All tests in this series involved introducing one or more reactants into the pool. The rate at which the reactions occur is controlled by the amounts of reactants present in a given time step. Therefore, the reaction rate was controlled by the concentration of the reactant for which the injection rate was the slowest.

The results from these tests indicate that this option does not give trustworthy results. This is not too surprising because pool sources were used and the pool-source tests (PS series) suggest that problems occur when materials are introduced into or removed from the pool. Nonetheless, CONTAIN does appear to be handling the chemical reaction energy in a proper manner.

As with the pool-source option, the pool-chemistry option gives questionable results and should be used with caution.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: PC01 - PC07 USER NAME: F. W. SCIACCA
2. TEST LEVEL: TL4A
3. TITLE OF TEST: POOL CHEMISTRY
4. CODE VERSION (DATE): A20 (11-1-82 THRU 12-3-82)
5. ACTIVE MODULES OR OPTIONS: POOL SOURCES, POOL CHEMISTRY, POOL THERMODYNAMICS, AND ATMOSPHERE THERMODYNAMICS
6. CONTAINMENT CONFIGURATION AND SOURCES: A SINGLE CELL WAS USED. IT CONTAINED A SODIUM ATMOSPHERE AND A SODIUM POOL. DIFFERENT MATERIALS WERE INTRODUCED INTO THE POOL AS CHEMICAL REACTANTS. DIFFERENT CHEMICAL REACTIONS WERE SPECIFIED. INITIAL POOL SIZES OF 500 M**3 AND 100 M**3 WERE USED.
7. TEST: HAND CALCULATIONS WERE MADE TO PREDICT POOL HEATUP RATES AND TIME TO POOL BOILING. THESE RESULTS WERE COMPARED WITH THOSE FROM CONTAIN. SOME OF THE CHEMICAL REACTIONS INCLUDED POOL SODIUM AS A REACTANT; OTHER REACTIONS DID NOT. ALL REACTIONS SPECIFIED WERE EXOTHERMIC. THE FOLLOWING LIST INDICATES THE CHEMICAL REACTIONS AND THE REACTION ENERGIES SPECIFIED FOR THE TEST CASES:

TEST	CHEMICAL REACTION	REACTION ENERGY, KJ/KG-MOLE	POOL SIZE, M**3
PC01	1.0 AL2O3 + 4.0 NA -- 1.0 CAO + 2.0 NA2O	5.10E5	100
PC02	1.0 AL2O3 + 1.0 CO -- 1.0 CAO + 2.0 NA2O	5.10E5	500
PC03	1.0 AL2O3 + 4.0 NA -- 1.0 CAO + 2.0 NA2O	5.10E5	500

TEST	CHEMICAL REACTION	REACTION ENERGY, KJ/KG-MOLE	POOL SIZE, M**3
PC04	1.0 GRAPH + 1.0 NA -- 1.0 CONC	1.00E7	100
PC05	1.0 GRAPH + 1.0 NA -- 1.0 CONC	2.00E3	100
PC06	1.0 GRAPH + 1.0 NA -- 1.0 CONC	2.00E4	100
PC07	1.0 AL2O3 + 1.0 SIO3 -- 1.0 CAO	5.10E5	500

THE REACTIONS SPECIFIED ARE COMPLETELY ARBITRARY AND BEAR NO RESEMBLANCE TO REAL CHEMICAL REACTIONS. THEY DO SERVE TO TEST THE POOL CHEMICAL-REACTION ROUTINE.

8. RESULTS OF TEST: IN GENERAL, THE CONTAIN RESULTS FOR THIS TEST SERIES DID NOT AGREE WELL WITH THE RESULTS OF HAND CALCULATIONS. SPECIFIC RESULTS ARE AS FOLLOWS:

TEST	TEST PARAMETER	CALCULATION	CONTAIN
PC01	TIME TO POOL BOILING	772 S	760 S
PC02	" " " "	3133 S	3880 S
PC03	" " " "	3860 S	3715 S
PC04	" " " "	18376 S	18250 S
PC05	POOL TEMP AT 10000 S	837 K	981 K
PC06	TIME TO POOL BOILING	WILL NOT BOIL	10710 S
PC07	" " " "	3029 S	4480 S

TESTS PC02, PC04 AND PC07 SHOWED REASONABLE AGREEMENT BETWEEN THE CONTAIN RESULTS AND THOSE FROM THE HAND CALCULATIONS. FOR THE OTHER TESTS, THE DIFFERENCES IN THE RESULTS RANGED FROM ABOUT 25% TO OVER 200%. THE DISAGREEMENT IS NOT TOO SURPRISING SINCE THE POOL-SOURCE TESTS (PS01 - PS11) INDICATED PROBLEMS WITH THE POOL HEAT BALANCES INVOLVING SOURCE MATERIALS. ALL OF THE POOL CHEMICAL-REACTION TESTS INVOLVED SOURCE MATERIALS.

TEST PC04 WAS SPECIFICALLY DESIGNED TO TEST THE CODE'S HANDLING OF THE CHEMICAL-REACTION ENERGY. THIS TEST EMPLOYED LARGE REACTION ENERGIES AND SMALL AMOUNTS OF REACTANT SOURCES. THE AGREEMENT BETWEEN THE CODE AND HAND CALCULATION RESULTS WAS VERY GOOD FOR THIS TEST. THIS INDICATES THAT THE HANDLING OF THE REACTION ENERGY FOR POOL CHEMICAL REACTIONS IS DONE CORRECTLY BY THE CODE. FOR THIS TEST, THE SUSPECTED ERRORS INTRODUCED BY SOURCE- AND SINK-ENERGY ACCOUNTING WERE KEPT VERY SMALL BY THE USE OF RELATIVELY SMALL REACTANT SOURCE RATES.

9. COMMENTS: CURRENTLY, THE POOL CHEMISTRY ROUTINE IN CONTAIN IS NOT VERY TRUSTWORTHY. THE DISAGREEMENT BETWEEN CONTAIN AND HAND-CALCULATED RESULTS VARIES FROM VERY SMALL TO FACTORS OF FOUR OR SO FOR THE TESTS RUN THUS FAR. THE TESTING-TO-DATE INDICATES THAT THE CODE'S HANDLING OF THE CHEMICAL REACTION ENERGY IS SOUND. THE PROBLEMS APPEAR TO BE ASSOCIATED WITH THE ENERGY BALANCE DURING SOURCE AND SINK MATERIALS.

EARLY IN THIS TEST SERIES, THE TEST RESULTS DEMONSTRATED THE NEED TO USE A MORE STRINGENT VOLUME-FRACTION CRITERION FOR POOL SOURCES THAN IS CURRENTLY USED IN THE UNMODIFIED CONTAIN CODING. THIS CRITERION IS USED TO DETERMINE WHICH MATERIALS IN THE POOL SHOULD BE TAKEN INTO ACCOUNT IN THE POOL HEAT

BALANCE AND WHICH SHOULD BE IGNORED. THE CURRENT VOLUME-FRACTION LIMIT BELOW WHICH MATERIALS ARE IGNORED IS 1.0E-6. EVEN AT THIS LIMIT, POOR HEAT BALANCES WERE OBTAINED. THE VOLUME-FRACTION LIMIT WAS REDUCED TO 1.0E-10 IN ALL OF THE TESTS NOTED ABOVE. THIS IMPROVED THE RESULTS BUT DID NOT SOLVE ALL OF THE PROBLEMS. THE DEFAULT VOLUME-FRACTION CRITERION FOR POOL MATERIALS SHOULD BE MADE MUCH LESS THAN THE CURRENT VALUE OF 1.0E-6.

THE CURRENT CODE-INPUT ROUTINES REQUIRE THAT AT LEAST TWO REACTION PRODUCTS BE SPECIFIED IN THE CHEMICAL-REACTION EQUATIONS GIVEN IN THE INPUT; OTHERWISE, SUBSEQUENT INPUT DATA ARE MISREAD. WHEN A SINGLE REACTION PRODUCT WAS DESIRED, THE INPUT PROBLEM WAS CIRCUMVENTED BY SPECIFYING 0.0 FOR THE NUMBER OF MOLES OF AN ARBITRARY SECOND REACTION PRODUCT.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

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1. PROBLEM: ID NO. PC01-01 2. LEVEL: PL3 3. RESOLVED? NO
4. DESCRIPTION: POOL HEAT BALANCES APPEAR TO BE IN ERROR. THE PROBLEM APPEARS TO BE IN THE SOURCE AND SINK THERMODYNAMICS OF THE POOL. THIS AFFECTS ANY TEST PROBLEMS THAT ATTEMPT TO USE THE POOL-CHEMISTRY ROUTINE.
5. DATE PROBLEM RESOLVED:

Supporting Analysis: PC Series - Pool Chemistry

CONTAIN will handle arbitrary chemical reactions. The reaction rates are specified by the rates at which the reactants enter the pool. In these tests, reactants were introduced into the pool at fixed rates for specified periods of time. In addition, for this check calculation it was assumed that the pool fluid was one of the reactants.

The chemical-reaction routine in CONTAIN requires that the user specify the energy associated with each reaction. The routine assumes that the pool reactions take place at the pool temperature. Therefore, standard energies of reaction should be adjusted to this temperature to obtain the proper user-specified reaction energies. To make these adjustments, preliminary hand calculations are used to estimate the pool temperature.

The heat of reaction for each chemical reaction can be determined from the standard heats of formation of the products minus the heats of formation of the reactants

$$\Delta H^{o}_{T_o} = H^{o}_{products} - H^{o}_{reactants} \qquad (3.5\text{-}16)$$

The heats of reaction can be adjusted using the following relationship:

$$\Delta H^{o}_{T} = \Delta H^{o}_{T_o} + \int_{T_o}^{T} (C_{p(products)} - C_{p(reactants)})dT \qquad (3.5\text{-}17)$$

where

C_p = specific heat of materials
T = pool temperature

The pool-chemistry tests employed an adiabatic pool. Energy is provided to or removed from the pool in the form of the heat carried in with the source material, the heat due to chemical reactions, and the heat carried out by any materials leaving the pool.

The pool energy balance is

Energy In - Energy Out = Change in Stored Energy
= Final Energy - Initial Energy

or

$$Q_{in} - Q_{out} = Q_{final} - Q_{initial}$$

For this analysis, assume the following chemical reaction:

$$\eta_{R_1} R_1 + \eta_{R_2} R_2 \rightarrow \eta_{P_1} P_1 \qquad (3.5\text{-}18)$$

where R_1 represents the reactant introduced into the pool, R_2 represents the pool fluid, and P_1 represents the reaction product. Then

$$Q_{in} = Q_{R_1} + \dot{Q}_{reac}t = (\dot{m}tC_pT_i)_{R_1} + \dot{Q}_{reac}t \qquad (3.5\text{-}19)$$

where $\dot{Q}_{reac}$ is the chemical-reaction heat-input rate, and $(\dot{m}tC_pT_i)_{R_1}$ represents the energy entering the pool with the reactant R_1 at temperature T_i (which may differ from the initial pool temperature). In this analysis nc material is removed from the pool. So

$$Q_{out} = 0 \qquad (3.5\text{-}20)$$

Because

$$Q_{final} = [(m - \dot{m}t)C_pT]_{R_2} + [\dot{m}tC_pT]_{P_1} \qquad (3.5\text{-}21)$$

and

$$Q_{initial} = (mC_pT_i)_{R_2} \ , \qquad (3.5\text{-}22)$$

the heat balance equation becomes

$$\dot{Q}_{reac}t + (\dot{m}tC_pT_i)_{R_1} = [(m - \dot{m}t)C_pT]_{R_2} + (\dot{m}tC_pT)_{P_1} - (mC_pT_i)_{R_2} \qquad (3.5\text{-}23)$$

This equation can be solved directly for the temperature, T, as a function of time, t. Alternatively, it can be used to calculate the time at which the pool reaches a given temperature.

3.5.5 Series PF - Sodium-Pool Fires

The treatment of a sodium-pool fire in CONTAIN was based on the SOFIRE-II burning models. The PF tests compared the CONTAIN results with results obtained from SOFIRE-II and with experimental results.

The early sodium-fire tests indicated that the CONTAIN results did not agree very well with other available results. Checks of the coding in CONTAIN revealed several errors. These were corrected to correspond to the models in SOFIRE-II. The updated coding gave good results for initial burning rates. However, with the model used in these tests, the burning rate decreased fairly rapidly. This behavior is not consistent with the results of experiments or with results obtained using SOFIRE-II.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: PF01 THRU PF04 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL5

3. TITLE OF TEST: SODIUM-POOL FIRES

4. CODE VERSION (DATE): 501 (5-82 THRU 8-12-82) AND 809 (8-19 THRU 8-31-82)

5. ACTIVE MODULES OR OPTIONS: SODIUM-POOL FIRE, ATMOSPHERE THERMODYNAMICS, HEAT TRANSFER

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE AIR-FILLED CELL CONTAINING A SODIUM POOL. SOME OF THE SPECIFIC TEST CONDITIONS ARE AS FOLLOWS:

TEST	POOL AREA M**2	POOL DEPTH M	GAS VOLUME M**3
PF01	0.557	0.0498	62.3
PF02	4.000	0.0920	400.0
PF03	4.000	1.0	400.0
PF04	10.000	1.5	10000.0

   TEST PF01 WAS INTENDED TO DUPLICATE SODIUM-POOL-FIRE TEST #4 (REF 1). TEST PF02 SIMULATED THE FRENCH CASSANDRE-POOL-FIRE TEST #8 (REF 2). TESTS PF03 AND PF04 ARBITRARILY EMPLOYED DEEPER POOLS. HEAT STRUCTURES SIMULATING THE TEST VESSEL WALLS WERE EMPLOYED IN EACH TEST. TESTS WERE RUN WITH POOL-TO-ATMOSPHERE AND ATMOSPHERE-TO-STRUCTURES HEAT TRANSFER ON AND OFF TO TEST THE EFFECTS OF THESE MODES OF ENERGY TRANSFER.

7. TEST: COMPARE THE SODIUM BURNING RATES PREDICTED BY CONTAIN WITH THE BURNING RATES OBTAINED FROM EXPERIMENTAL RESULTS. ALSO COMPARE THE CONTAIN RESULTS WITH PREDICTIONS FROM HAND CALCULATIONS USING THE SOFIRE-II ANALYSIS METHODS.

8. RESULTS OF TEST: THE CONTAIN RESULTS FOR BURNING RATES ARE SUBSTANTIALLY LOWER THAN THE EXPERIMENTAL BURNING RATES FOR SODIUM-POOL FIRES. THE CONTAIN RATE FROM PF01 WAS ON THE ORDER OF 4.5

KG/M**2-HR, WHEREAS THE CORRESPONDING TEST RESULTS FOR "TEST 4" REPORTED IN AI-AEC-13055 RANGED FROM 24 TO 34 KG/M**2-HR. IN ADDITION, THE CONTAIN SIMULATION OF CASSANDRE TEST #8 GAVE BURNING RATES OF ABOUT 3.5 KG/M**2-HR. THE EXPERIMENTAL RATES VARIED WITH TIME BUT HAD AN AVERAGE VALUE OF ABOUT 17.7 KG/M**2-HR.

9. COMMENTS: THE ORIGINAL CODING IN CONTAIN VERSIONS 501 AND 809 GAVE SODIUM-POOL-FIRE BURNING RATES THAT ARE ABOUT A FACTOR OF FIVE OR MORE LOWER THAN THE SODIUM BURNING RATES OBTAINED FROM EXPERIMENTAL RESULTS. THIS CODING WAS BASED ON THE ANALYTICAL BURNING MODEL USED IN THE SOFIRE-II CODE. CHECKS OF THE POOL-FIRE SUBROUTINE IN CONTAIN REVEALED SEVERAL CODING ERRORS WHEN COMPARED TO THE SOFIRE-II MODEL. THESE WERE CORRECTED VIA UPDATE "MODFIRE". THE RESULTS USING THIS UPDATE ARE DISCUSSED IN THE TEST REPORT FOR TEST PF05.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

REF 1. AI-AEC-13055, SOFIRE II USER REPORT, P. BEIRINGER, ET AL, ATOMICS INTERNATIONAL, 1973.

REF 2. MALET, J.C., ET AL, POTENTIAL RESULTS OF SPRAY AND POOL FIRES, NUCLEAR ENGINEERING AND DESIGN, 68(1981).

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1. PROBLEM: ID NO. PF01-01 2. LEVEL: PL 3 3. RESOLVED? NO
4. DESCRIPTION: THE CONTAIN SODIUM-POOL-FIRE BURNING RATES ARE A FACTOR OF FIVE OR MORE LOWER THAN EXPERIMENTAL RATES.
5. DATE PROBLEM RESOLVED:

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CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: PF05 USER NAME: F. W. SCIACCA

2. TEST LEVEL: TL4A, TL5

3. TITLE OF TEST: SODIUM-POOL FIRES

4. CODE VERSION (DATE): 809, WITH UPDATES (9-23-82)

5. ACTIVE MODULES OR OPTIONS: SODIUM-POOL FIRE, ATMOSPHERE THERMODYNAMICS, HEAT TRANSFER

6. CONTAINMENT CONFIGURATION AND SOURCES: SINGLE AIR-FILLED CELL CONTAINING A SODIUM POOL. THE SPECIFIC TEST CONDITIONS ARE AS FOLLOWS:

POOL AREA M**2	POOL DEPTH M	GAS VOLUME M**3
4.000	1.0	400.0

TEST PF05 SIMULATED THE FRENCH CASSANDRE-POOL-FIRE TEST #8 (REF 1). THIS TEST WAS SIMILAR TO PF02 BUT EMPLOYED A DEEPER POOL. NO HEAT STRUCTURES WERE INCLUDED IN THE CALCULATION. ALL POOL HEAT TRANSFER WAS TURNED OFF.

7. TEST: COMPARE THE SODIUM BURNING RATES PREDICTED BY CONTAIN WITH THE BURNING RATES OBTAINED FROM EXPERIMENTAL RESULTS. ALSO, COMPARE THE CONTAIN RESULTS WITH PREDICTIONS FROM HAND CALCULATIONS USING THE SOFIRE-II ANALYSIS METHODS. OTHER PARAMETERS COMPARED ARE THE POOL AND ATMOSPHERE HEATUP AT SELECTED TIMES.

8. RESULTS OF TEST: THE CASSANDRE #8 TEST REPORTEDLY HAD AN AVERAGE BURNING RATE OF 17.7 KG/M**2-HR. TEST PF05 GAVE AN INITIAL SODIUM BURNING RATE WHICH WAS QUITE CLOSE TO THIS. HOWEVER, THE CONTAIN BURNING RATES DROP OFF SIGNIFICANTLY WITH TIME, AS INDICATED BELOW.

TIME, S	BURNING RATE, KG/M**2-HR
1000	16.09
1500	14.15
2000	11.81
2500	8.81

THUS, CONTAIN'S PREDICTION OF BURNING RATE IS QUITE GOOD AT THE BEGINNING OF A PROBLEM. ITS PREDICTIONS FOR LATER TIMES DEVIATE SIGNIFICANTLY FROM RATES OBSERVED IN THE EXPERIMENT BEING MODELED.

POOL AND ATMOSPHERE HEAT BALANCE CHECKS WERE ALSO MADE. THE DEFAULT POOL-FIRE MODEL IN CONTAIN ALLOTS HALF OF THE CHEMICAL REACTION HEATING FROM THE POOL FIRE TO THE SODIUM POOL AND HALF TO THE CELL ATMOSPHERE. HAND CALCULATIONS WERE MADE OF THE POOL AND ATMOSPHERE HEATING. THESE CALCULATIONS USED AS INPUT THE TOTAL OXYGEN CONSUMED (AS PREDICTED BY CONTAIN) UP TO A SELECTED TIME. THE RESULTS OF THESE CHECKS ARE AS FOLLOWS:

TEST PARAMETER	CALCULATED	CONTAIN
SODIUM POOL TEMP RISE (K) UP TO 3132 S	59.6	61.2
CELL ATMOSPHERE TEMP RISE (K) UP TO 3132 S	630.5	613.9

THESE NUMBERS SHOW REASONABLE AGREEMENT. THUS, CONTAIN APPEARS TO BE DOING A REASONABLE JOB OF HANDLING THE ENERGY FROM A SODIUM POOL FIRE.

THE ATMOSPHERE AND POOL TRENDS PREDICTED BY CONTAIN FOR TEST PF05 ARE DISPLAYED IN FIGURES PF-01 THROUGH PF-05. FIGURE PF-01 SHOWS THE ATMOSPHERE TEMPERATURE CHANGE WITH TIME. NEAR THE END OF THE CALCULATION THE PLOT FLATTENS OUT BECAUSE OF THE DECREASE IN THE REACTION RATE. FIGURE PF-02 SHOWS THE OXYGEN CONCENTRATION VS TIME. THE POOL TEMPERATURE CHANGE IS SHOWN IN FIGURE PF-03. BOTH OF THESE PLOTS ALSO SHOW THE EFFECTS OF THE DECREASING REACTION RATE. THE SODIUM-OXYGEN REACTION PRODUCES AEROSOLS OF NA2O AND NA2O2. THE BUILDUP OF AEROSOLS IN THE CELL ATMOSPHERE IS ILLUSTRATED IN FIGURE PF-04. THIS BUILDUP PEAKS AT ABOUT 3000 SECONDS IN THIS CALCULATION. THE PEAKING AT THIS

TIME IS DUE BOTH TO THE DECREASE IN THE REACTION RATE AND THE EFFECTS OF AEROSOL DEPOSITION. FIGURE PF-05 SHOWS THE CUMULATIVE AEROSOL DEPOSITION WITH TIME.

9. COMMENTS: THE ORIGINAL CODING IN CONTAIN VERSIONS 501 AND 809 GAVE SODIUM-POOL-FIRE BURNING RATES THAT WERE ABOUT A FACTOR OF FIVE OR MORE LOWER THAN THE SODIUM BURNING RATES OBTAINED FROM EXPERIMENTAL RESULTS. THIS CODING WAS BASED ON THE ANALYTICAL BURNING MODEL USED IN THE SOFIRE-II CODE (REF 2). CHECKS OF THE POOL-FIRE SUBROUTINE IN CONTAIN REVEALED SEVERAL CODING ERRORS WHEN COMPARED TO THE SOFIRE-II MODEL. THESE WERE CORRECTED VIA UPDATE "MODFIRE". THE UPDATED VERSION OF THE CODE NOW GIVES INITIAL BURNING RATES THAT ARE IN GOOD AGREEMENT WITH THOSE OBTAINED IN EXPERIMENTS. LATER-TIME BURNING RATES ARE NOT IN GOOD AGREEMENT WITH EXPERIMENTAL RESULTS.

A CHECK OF THE BURNING-RATE CALCULATION IN CONTAIN (BASED ON THE SOFIRE-II CODE) INDICATED THAT THE RATE IS DEPENDENT ON THE TEMPERATURE DIFFERENCE BETWEEN THE POOL SURFACE AND THE ATMOSPHERE. IN THIS PARTICULAR TEST THE ATMOSPHERE MASS WAS RELATIVELY SMALL AND HEATED UP MUCH FASTER THAN THE SODIUM POOL. THE TEMPERATURE DIFFERENTIAL BETWEEN THE GAS AND THE POOL SURFACE THUS DECREASES WITH TIME. THIS, IN TURN, REDUCES THE BURNING RATE. THIS MODEL DOES NOT APPEAR TO BE A VALID REPRESENTATION OF ACTUAL BURNING PHENOMENA. A MORE SUITABLE MODEL SHOULD BE PROVIDED.

10. SUGGESTIONS FOR ADDITIONAL TESTS: NONE.

REF 1. MALET, J.C., ET AL, POTENTIAL RESULTS OF SPRAY AND POOL FIRES, NUCLEAR ENGINEERING AND DESIGN, 68(1981).

REF 2. AI-AEC-13055, SOFIRE II USER REPORT, P. BEIRINGER, ET AL, ATOMICS INTERNATIONAL, 1973.

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1. PROBLEM: ID NO. PF05-01   2. LEVEL: PL 3   3. RESOLVED? NO
4. DESCRIPTION: THE CONTAIN SODIUM-POOL-FIRE BURNING RATES DO NOT MATCH THOSE REPORTED IN EXPERIMENTAL WORK.
5. DATE PROBLEM RESOLVED:

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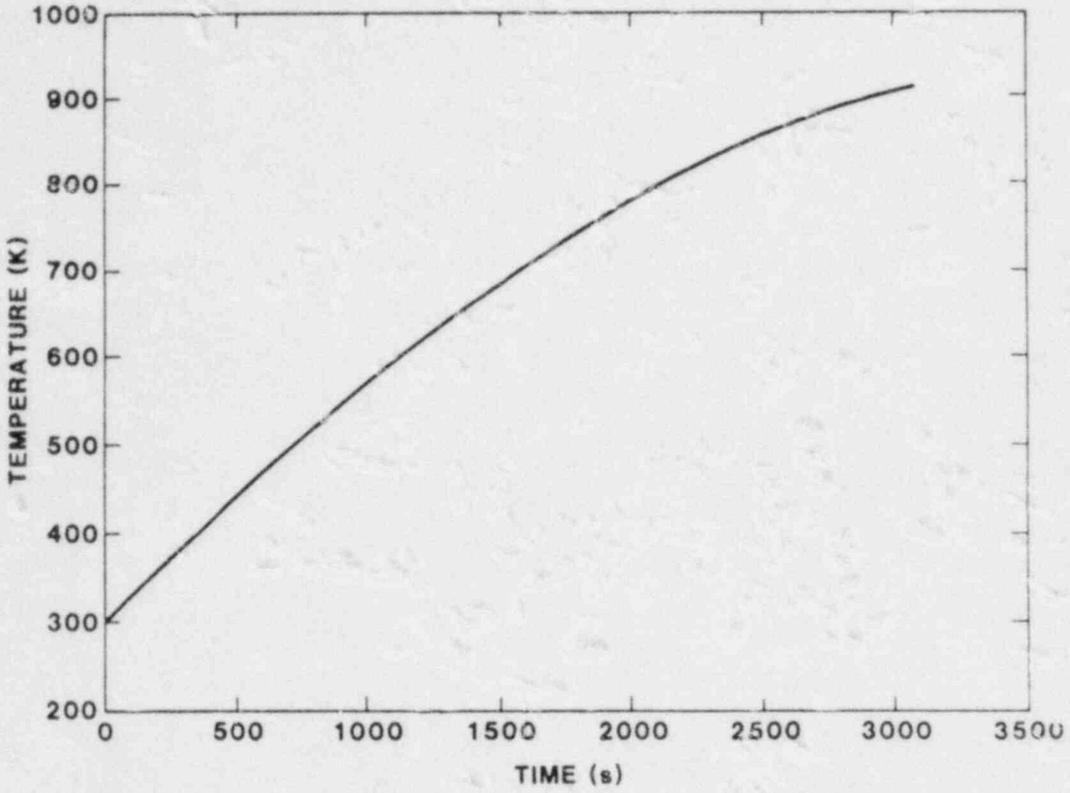

Figure PF-01 Cell gas temperature during sodium-pool fire (Test PF05).

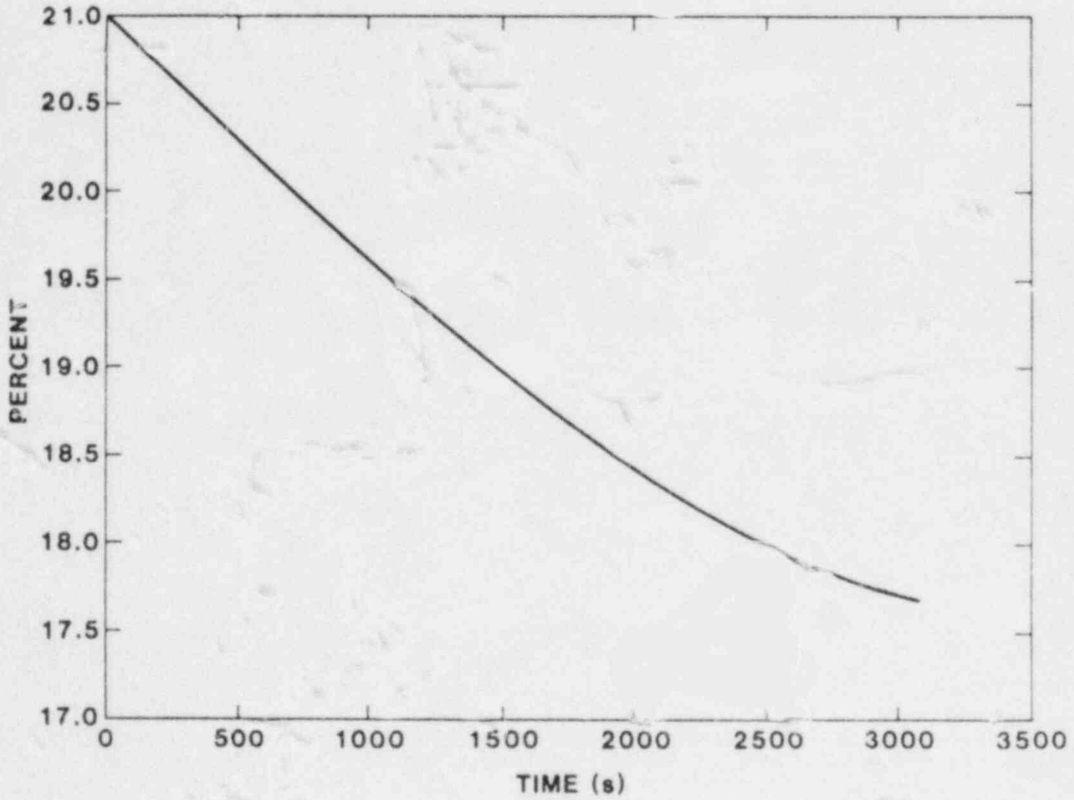

Figure PF-02 Concentration of oxygen in cell atmosphere during sodium-pool fire (Test PF05).

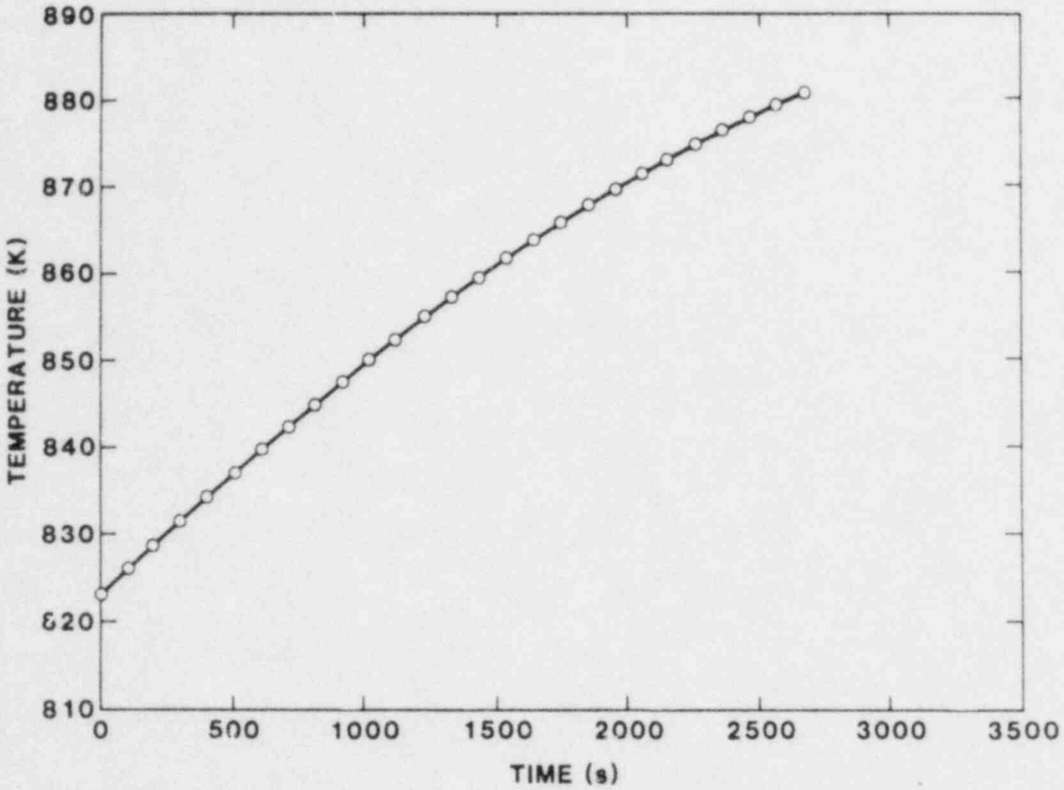

Figure PF-03 Temperature of sodium-pool during sodium-pool fire (Test PF05).

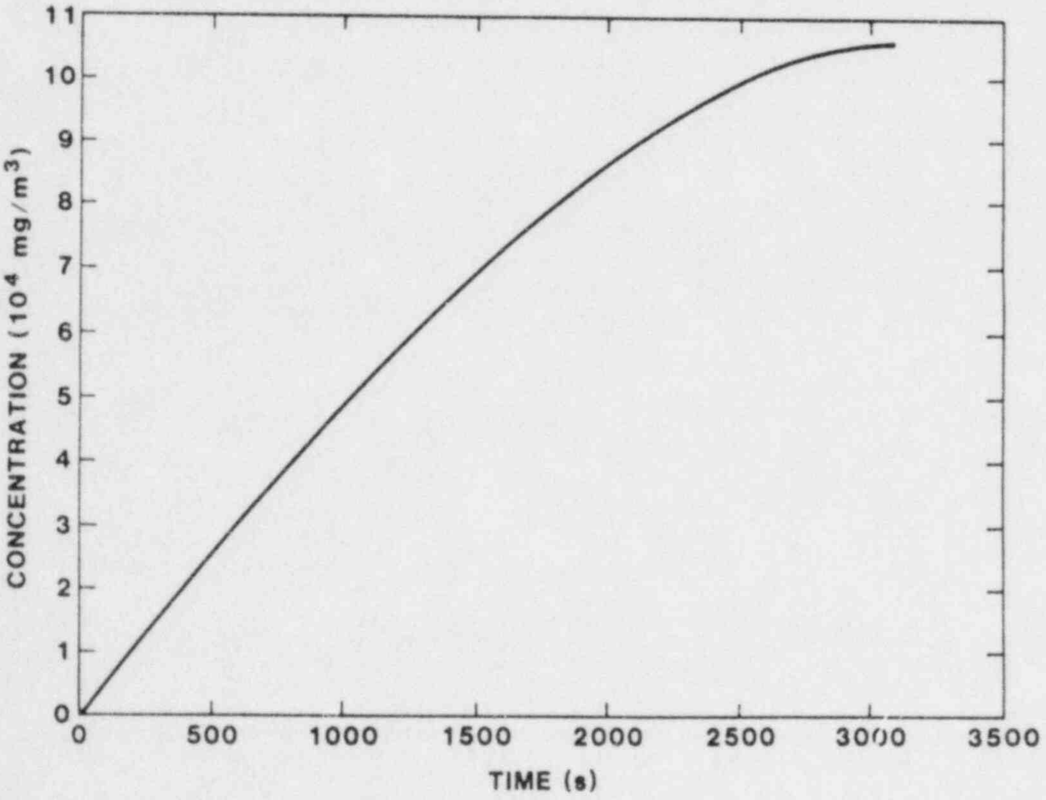

Figure PF-04 Concentration of aerosols (Na_2O plus Na_2O_2) in atmosphere during sodium-pool fire (Test PF05).

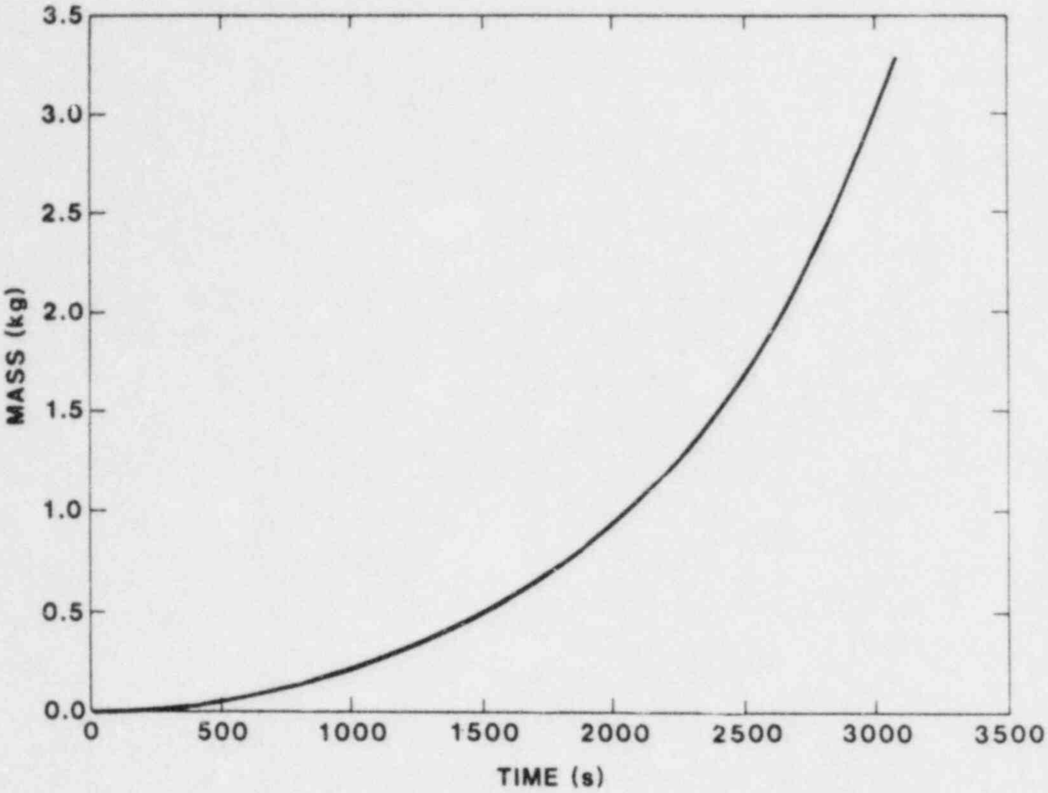

Figure PF-05 Total mass of aerosols deposited during sodium-pool fire (Test PF05).

Supporting Analysis: PF Series - Sodium-Pool Fire

Sodium reacts with oxygen according to the following reaction equations:

$$F\ (4.0\ Na + 1.0\ O_2) \rightarrow F\ (2\ Na_2O + 2\ Q_{mon}) \qquad (3.5\text{-}24)$$

$$(1 - F)(2.0\ Na + 1.0\ O_2) \rightarrow (1 - F)(Na_2O_2 + Q_{per}) \qquad (3.5\text{-}25)$$

where F is the fraction of oxygen consumed that goes into the formation of sodium monoxide (Na_2O), Q_{mon} is the heat of reaction resulting from the formation of Na_2O, and Q_{per} is the heat of reaction resulting from the formation of Na_2O_2.

The above equations can be added to give

$$(1 + F)2Na + O_2 \rightarrow (2F)Na_2O + (1 - F)Na_2O_2 + (2F)Q_{mon} + (1 - F)Q_{per} \qquad (3.5\text{-}26)$$

The heats of reaction are (Ref. 1):

$$Q_{mon} = 3900\ \text{Btu/lb Na} = 9.08 \times 10^6\ \frac{J}{kg\ Na} \qquad (3.5\text{-}27)$$

$$Q_{per} = 4500\ \text{Btu/lb Na} = 10.48 \times 10^6\ \frac{J}{kg\ Na} \qquad (3.5\text{-}28)$$

There are 2 x 23 = 46 kg of Na per kg-mole of either Na_2O or Na_2O_2. In terms of the amount of oxygen consumed, the heat of reaction can be expressed as follows:

$$Q_{reac} = \left[2 \times \frac{F \times 46 \times Q_{mon}}{\text{kg-mole } O_2} + \frac{(1 - F) \times 46 \times Q_{per}}{\text{kg-mole } O_2} \right] \times \eta_{O_2} \qquad (3.5\text{-}29)$$

where η_{O_2} is the total number of kg-moles of oxygen consumed in the reaction.

In these check calculations, the evaluation concentrated on the total energy produced in the sodium-pool fire and the partitioning of this energy between the sodium pool and the cell atmosphere above the pool. Checks of burning rates were made by comparing CONTAIN predictions with actual test results and are not included here.

These check calculations utilized the total oxygen consumption as predicted by CONTAIN. In addition, the value of F was taken to be 0.5 (half of the O_2 consumed went into the formation of Na_2O and half went into the formation of Na_2O_2). It was also assumed that one-half of the reaction energy went into the sodium pool, and the other half went into atmospheric heating. The pool and atmosphere were adiabatic, and there were no heat sources (or sinks) other than the O_2-Na reaction. These assumptions are consistent with those used in the CONTAIN tests.

For a given test, the amount of O_2 consumed up to a selected time is η_{O_2}. The total reaction energy generated is calculated from Equation (3.5-29). Of this, half goes into heating of the Na pool.

The pool heat balance is

$$Q_{in} - Q_{out} = Q_{final} - Q_{initial}$$

where, as assumed, $Q_{out} = 0$.

If the reaction products (Na_2O and Na_2O_2) are ignored in the heat balance, then

$$0.5\ Q_{reac} - 0 = M_{Na_f} C_p T_f - M_{Na_i} C_p T_i \qquad (3.5\text{-}30)$$

and

$$\Delta T = T_f - T_i = \frac{0.5\ Q_{reac} + M_{Na_i} C_p T_i}{M_{Na_f} C_p} - T_i \qquad (3.5\text{-}31)$$

where

M_{Na} = sodium mass
C_p = sodium specific heat (average for the range T_i to T_f)
f denotes final conditions
i denotes initial conditions

The atmosphere heat balance is similar:

$$Q_{in} - Q_{out} = Q_{final} - Q_{initial}$$

$$0.5\ Q_{reac} - 0 = M_{A_f} C_{v_A} T_f - M_{A_i} C_{v_A} T_i \qquad (3.5\text{-}32)$$

$$\Delta T = \frac{0.5\ Q_{reac} + M_{A_i} C_{v_A} T_i}{M_{A_f} C_{v_A}} - T_i \qquad (3.5\text{-}33)$$

where A denotes atmosphere conditions.

3.5.6 Pool-Model Revisions

The several test series concerned with pool-related phenomena have identified a number of deficiencies. As indicated by the problem reports, many of these problems had not been resolved at the time of publication of this report. The reason for this is that a major revision of the reactor cavity and pool models was undertaken. This revision was prompted not only by the problems identified by the tests but also by a reassessment of the level of analysis appropriate to reactor cavity models. At the time of writing, this revision was not complete, but when it is, the code will be thoroughly subjected to the tests described here and, no doubt, to other tests.

3.6 AEROSOL-BEHAVIOR TESTS

Tests AB01 through AB03 provide CONTAIN predictions of aerosol behavior that are compared with the results obtained from experiments and from other codes. The comparisons show that CONTAIN does an excellent job of modeling aerosol behavior. Because of the complex nature of aerosol processes, no separate supporting analysis is provided. However, the basis for comparisons made is adequately described in the Test Summary Reports. In addition, all updates used in making the CONTAIN runs are presented with the Input Data Sets.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: AB01(ST) USER NAME: K. K. MURATA
2. TEST LEVEL: TL2, TL3
3. TITLE OF TEST: DRY URANIUM OXIDE AEROSOL EXPERIMENT COMPARISON (NSPP 207)
4. CODE VERSION (DATE): 809 (9/24/82)
5. ACTIVE MODULES OR OPTIONS: AEROSOL MODULE
6. CONTAINMENT CONFIGURATION AND SOURCES: THE CONFIGURATION MODELED WAS THE ORNL NSPP VESSEL. THE AEROSOL BEHAVIOR WAS CALCULATED USING AN INITIAL CONDITION CORRESPONDING TO THAT MEASURED EXPERIMENTALLY.[1] THE INITIAL PARTICLE SIZE DISTRIBUTION WAS ASSUMED TO BE LOGNORMAL. THE TEMPERATURE AND PRESSURE OF THE VESSEL WERE ASSUMED CONSTANT. THE INITIAL CONDITIONS WERE TAKEN AFTER THE SOURCE-INPUT PERIOD AT 25.8 MINUTES; THEREFORE, NO SOURCES WERE INTRODUCED DURING THE CALCULATION.
7. TEST: THE CONTAIN-CALCULATED AEROSOL MASS CONCENTRATION IS COMPARED BOTH WITH EXPERIMENTAL RESULTS AND WITH A HAARM-3 BEST FIT TO THE EXPERIMENT. SHAPE FACTORS WERE ADJUSTED TO OBTAIN THE CONTAIN BEST FIT TO THE EXPERIMENT. IN ADDITION, RESULTS USING THE SAME SHAPE FACTORS AS USED IN THE HAARM-3 BEST FIT ARE GIVEN.[2] THE CONTAIN TEST IS AT BEST QUALITATIVE AND CHECKS CONSISTENCY (LEVELS TL2 AND TL3) SINCE ADJUSTMENT OF SHAPE FACTORS WAS ALLOWED. THE RANGE OF VARIATION ALLOWED BY VARYING SHAPE FACTORS IS SUFFICIENTLY LARGE THAT THE FITTING PROCEDURE MAY MASK CODING ERRORS AND INADEQUATE MODELING. THE COMPARISON TO HAARM-3 IS MADE, BUT BECAUSE OF THE LOGNORMAL ASSUMPTION MADE IN HAARM-3, ONE WOULD NOT EXPECT THE RESULTS TO AGREE. THE CONTAIN BEST FIT APPEARS TO BE SOMEWHAT BETTER THAN THE HAARM-3 BEST FIT. A CHECK ON MASS CONSERVATION IN THE CONTAIN CALCULATION IS MADE.
8. RESULTS OF TEST: FIGURE AB-01 SHOWS THREE SETS OF CODE CALCULATIONS STARTING AT 25.8 MINUTES WITH A MASS CONCENTRATION OF 3.43 G/M^3. IN THE HAARM-3 CALCULATION AND IN CONTAIN RUN A, A DYNAMIC SHAPE FACTOR VALUE OF CHI = 3 AND AN AGGLOMERATION SHAPE FACTOR VALUE OF GAMMA = 10 WERE USED. THE CONTAIN BEST FIT, RUN B, USED CHI = 1.5 AND GAMMA = 7. BECAUSE

THE AERODYNAMIC MEDIAN RADIUS IS WHAT IS DETERMINED EXPERIMENTALLY, AND NOT THE MASS-EQUIVALENT RADIUS, THE DYNAMIC SHAPE FACTOR IS REQUIRED TO COMPUTE THE LATTER. THE CONTAIN BEST FIT SHAPE FACTOR GIVES AN INITIAL MASS-EQUIVALENT MEDIAN RADIUS OF .53 MICROMETERS. THE INITIAL GEOMETRIC STANDARD DEVIATION IS 3.8. MASS CONSERVATION WAS EXACT, AS IT SHOULD BE, SINCE THE CODE ADJUSTS FOR IT BY SUBTRACTING FROM THE DEPOSITED AEROSOL MASS. (THIS HAS BEEN CHANGED IN LATER VERSIONS.)

9. COMMENTS: THE AGREEMENT BETWEEN THE CONTAIN BEST FIT AND EXPERIMENT IS GOOD. THE HAARM-3 BEST FIT, WHEN COMPARED TO BOTH THE EXPERIMENTAL RESULTS AND TO THE CONTAIN BEST FIT, LIES TOO HIGH AT EARLY TIMES AND TOO LOW AT LATE TIMES. THIS OVERSHOOT/UNDERSHOOT IS CHARACTERISTIC OF LOGNORMAL CODES AFTER THE END OF THE SOURCE.[3] THE CONTAIN BEST FIT DOES NOT APPEAR TO REPRODUCE THE SLOPE OF THE MASS CONCENTRATION CURVE AT 25.8 MINUTES. THE DIFFICULTY IS PRESUMABLY RELATED TO THE LOGNORMAL ASSUMPTION FOR THE INITIAL PARTICLE DISTRIBUTION. WHETHER A DIFFERENT INITIAL DISTRIBUTION (CONSISTENT WITH THE SCATTER IN THE EXPERIMENTAL SIZE DISTRIBUTION DATA) WOULD GIVE A BETTER INITIAL SLOPE HAS NOT BEEN INVESTIGATED.

   NOTE THAT THIS TEST WAS RUN WITH AN UPDATE CORRECTION SET GIVEN IN THE INPUT-DATA-SET SECTION. FOR THE CODE VERSION USED, THERE WAS NO WAY TO CHANGE THE INTERNALLY SET AEROSOL PARAMETERS, EXCEPT THROUGH UPDATES. THIS WILL BE CHANGED IN LATER VERSIONS. A CODING ERROR, THE OMISSION OF THE DYNAMIC SHAPE FACTOR IN THE EXPRESSION FOR THE STOKES SETTLING VELOCITY, WAS DISCOVERED SHORTLY BEFORE THESE CALCULATIONS WERE PERFORMED, AND THE CORRECTION IS ALSO PART OF THE UPDATE SET.

10. SUGGESTIONS FOR ADDITIONAL TESTS: IN ORDER TO VERIFY THE NUMERICAL PROCEDURE USED IN THE AEROSOL MODULE, IT IS QUITE CLEAR THAT A COMPARISON TO A CODE LIKE QUICK,[4] WHICH ALLOWS A GENERAL INSTEAD OF LOGNORMAL REPRESENTATION OF THE SIZE DISTRIBUTION FUNCTION, IS REQUIRED. THESE COMPARISONS WILL BE THE SUBJECT OF UPCOMING TEST REPORTS.

11. REFERENCES AND BIBLIOGRAPHY:

1. Adams, R. E., T. S. Kress, and M. L. Tobias, "Sodium Oxide and Uranium Oxide Aerosol Experiments: NSPP Tests 106-108 and Tests 204-207, Data Record Report," NUREG/CR-1767, ORNL/NUREG/TM-408 (Oak Ridge, TN: Oak Ridge National Laboratories, 1981).

2. Adams, R. E., T. S. Kress, J. T. Han, and M. Silberberg, Behavior of Sodium Oxide, Uranium Oxide, and Mixed Sodium Oxide-Uranium Oxide Aerosols in a Large Vessel, Proceedings of the CSNI Specialists Meeting on Nuclear Aerosols in Reactor Safety, NUREG/CR-1724, ORNL/NUREG/TM-404 CSNI-45, Gatlinburg, TN, April 1980.

3. Jordan, H., P. M. Schumacher, J. A. Gieseke and K. W. Lee, Aerosol Behavior Modeling, op cit.

4. Jordan, H., P. M. Schumacher, and J. A. Gieseke, QUICK Users' Manual, NUREG/CR-2105, BMI-2082, Battelle Columbus Laboratories, May 1981.

5. Gelbard, F., "MAEROS User Manual," NUREG/CR-1391, SAND80-0822 (Albuquerque, NM: Sandia National Laboratories, 1982).

==

1. PROBLEM: ID NO. AB01-01 2. LEVEL: PL-2 3. RESOLVED? YES
4. DESCRIPTION: SHAPE FACTOR OMITTED FROM STOKES SETTLING VELOCITY.
5. DATE PROBLEM RESOLVED: 10/20/82

==

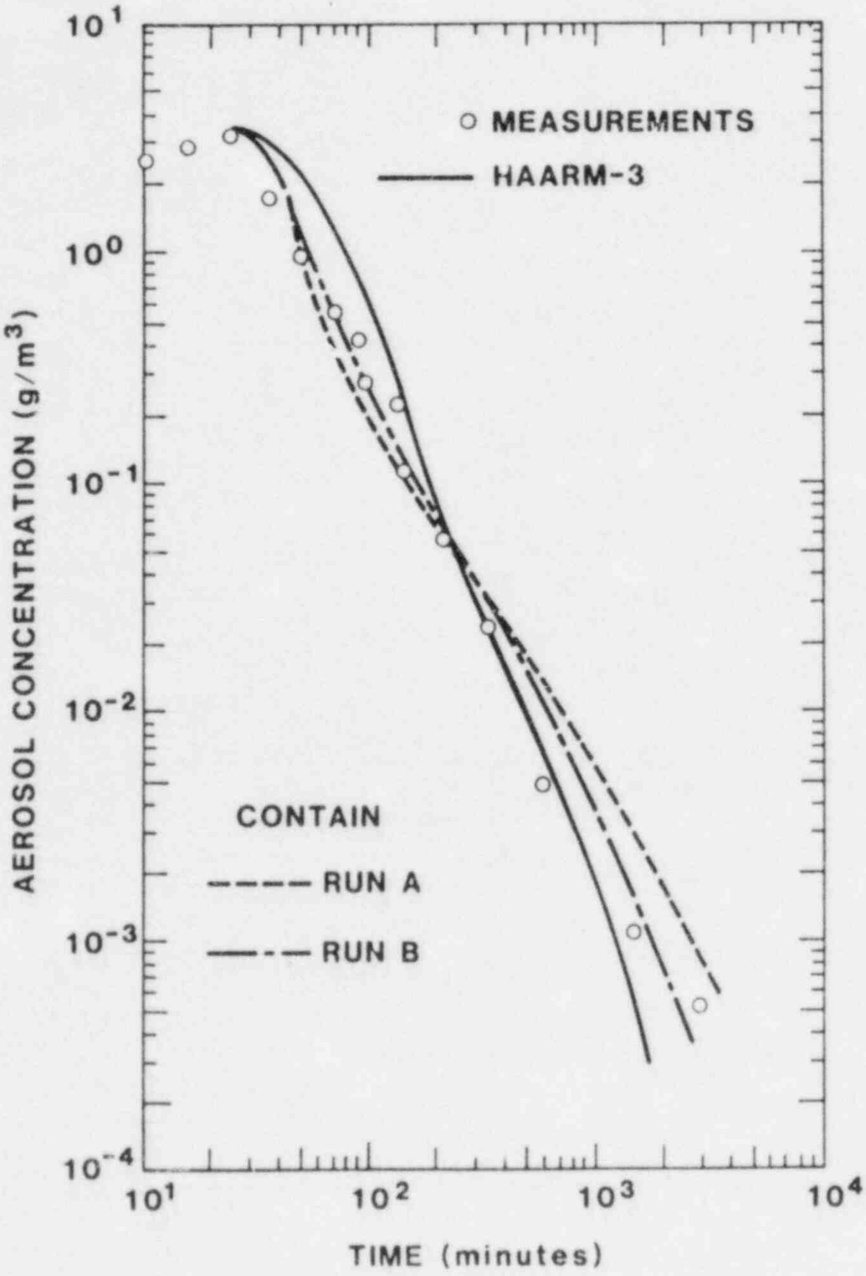

Figure AB-01 Comparison of HAARM-3 calculations and two CONTAIN calculations of aerosol concentration for experiment NSPP 207 (CONTAIN Test AB01).

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: AB02, AB03 USER NAME: K. K. MURATA

2. TEST LEVEL: TL4C

3. TITLE OF TEST: COMPARISON OF CONTAIN TO THE QUICK CODE FOR CONDITIONS CORRESPONDING TO THE CSTF-AB1 AND -AB3 EXPERIMENTS

4. CODE VERSION (DATE): 1020 (11/18/82)

5. ACTIVE MODULES OR OPTIONS: AEROSOL MODULE

6. CONTAINMENT CONFIGURATION AND SOURCES: THE PURPOSE OF THESE TESTS IS TO TEST THE CONTAIN AEROSOL-PHYSICS MODELING AND NUMERICAL SOLUTION SCHEME BY COMPARING RESULTS WITH THOSE FROM THE QUICK CODE.[1] THE CONFIGURATION IS A SINGLE-CELL MODEL OF THE HEDL CSTF VESSEL. HEAT TRANSFER AND ATMOSPHERE THERMODYNAMICS WERE NOT MODELED, ALTHOUGH A TIME-DEPENDENT TEMPERATURE GRADIENT AT THE VESSEL WALL WAS INTRODUCED THROUGH UPDATE CORRECTIONS. QUICK CALCULATIONS WERE AVAILABLE[2] FOR TWO SODIUM OXIDE AEROSOL EXPERIMENTS, WHICH WERE CONDUCTED UNDER CONSIDERABLY DIFFERENT CONDITIONS IN THE HEDL FACILITY: A SODIUM POOL FIRE TEST,[3] AB1, AND A SODIUM-SPRAY FIRE TEST,[4] AB3. THE SOURCE TERMS WERE THOSE USED IN QUICK CALCULATIONS[2] FOR AB1 AND AB3. COMPARISONS WITH THE QUICK RESULTS THAT FIT THE TWO EXPERIMENTS ARE PRESENTED. THE CONTAIN COMPARISON FOR THE AB1 EXPERIMENT CONSTITUTES CONTAIN TEST AB02, AND THAT FOR THE AB3 EXPERIMENT CONSTITUTES CONTAIN TEST AB03.

   IT SHOULD BE NOTED THAT THE PRESENT TEST IS PROBABLY AS MUCH A TEST OF QUICK AS IT IS OF CONTAIN, BECAUSE ANALYTIC RESULTS FOR COMPARISON PURPOSES ARE NOT AVAILABLE EXCEPT IN SPECIAL CASES THAT DO NOT EXERCISE MUCH OF THE PHYSICS MODELING.

7. TEST: THE CONTAIN CALCULATIONS WERE OF TWO TYPES: IN THE FIRST TYPE, CONTAIN WAS RUN WITH THE SOURCE TERMS AND AEROSOL-PHYSICS INPUT PARAMETERS USED IN THE QUICK CALCULATIONS. THE MAEROS AEROSOL-PHYSICS MODELING NORMALLY PRESENT IN CONTAIN WAS UTILIZED. THIS TYPE OF CALCULATION TESTS THE AEROSOL-PHYSICS MODELING AND THE NUMERICAL SOLUTION SCHEMES IN THE TWO CODES FOR THE SAME SET OF USER-DEFINED PHYSICS PARAMETERS. BOTH CODES USE DISCRETE OR SIZE-CLASS METHODS TO REPRESENT THE PARTICLE DISTRIBUTION FUNCTION. BUT, BECAUSE OF THE DIFFERENCES IN THE SOLUTION SCHEMES, THE SIZE-CLASS INPUT PARAMETERS IN THE CONTAIN CALCULATIONS WERE OPTIMIZED FOR CONTAIN AND ARE NOT THE SAME AS THOSE USED IN THE QUICK CALCULATIONS.

   THERE ARE SOMEWHAT SUBTLE DIFFERENCES IN THE QUICK AND THE CONTAIN (MAEROS) MODELING OF THE AEROSOL PHYSICS. FOR EXAMPLE, NON-STOKESIAN SETTLING VELOCITIES ARE USED IN QUICK BUT NOT IN CONTAIN. ALSO, IN QUICK, THE AGGLOMERATION SHAPE FACTOR IS USED TO SCALE THE SPHERICAL EQUIVALENT RADIUS IN SOME PLACES WHERE IT IS NOT SCALED IN CONTAIN, SUCH AS IN THE KNUDSEN NUMBER AND THERMOPHORETIC FORCE.

   IN THE SECOND TYPE OF CALCULATION, UPDATE CORRECTIONS WERE MADE IN CONTAIN TO CHANGE THE PHYSICS MODELING TO THAT USED IN QUICK. THE SOURCE TERMS AND

PHYSICS INPUT PARAMETERS WERE KEPT THE SAME. THE SECOND TYPE OF CALCULATION THUS PROVIDES A DIRECT COMPARISON OF THE NUMERICAL SOLUTION SCHEMES.

8. RESULTS OF TEST: THE RESULTS OF THE CALCULATIONS ARE SHOWN IN FIGURES AB-02 THRU AB-05. FIGURE AB-02 COMPARES THE QUICK CALCULATION AND THE TWO TYPES OF CONTAIN CALCULATIONS FOR THE MASS CONCENTRATION AS A FUNCTION OF TIME FOR CONTAIN TEST AB02. FIGURE AB-03 PROVIDES A COMPARISON OF THE AERODYNAMIC MASS MEDIAN DIAMETERS. THE EXPERIMENTAL DATA ARE ALSO SHOWN, EVEN THOUGH COMPARISON WITH EXPERIMENT IS NOT THE POINT OF THIS PARTICULAR TEST. THE AGREEMENT BETWEEN CODE RESULTS IS GOOD WHEN THE CONTAIN TYPE OF PHYSICS MODELING IS USED AND EXCELLENT WHEN THE CONTAIN PHYSICS MODELS (MAEROS MODELS) ARE CONVERTED TO THE QUICK MODELS.

   FIGURE AB-04 SHOWS THE COMPARISONS FOR THE MASS CONCENTRATION IN THE CONTAIN AB03 TEST, AND FIGURE AB-05 SHOWS THE COMPARISONS FOR THE AERODYNAMIC SETTLING DIAMETER. THE AGREEMENT IN THE MASS CONCENTRATION IS AGAIN GOOD WHEN THE CONTAIN TYPE OF MODELING IS USED AND EXCELLENT WHEN THE CONTAIN MODELS ARE CONVERTED TO QUICK MODELS. THE DISCREPANCY BETWEEN THE QUICK AND CONTAIN RESULTS FOR THE AERODYNAMIC SETTLING DIAMETER IS APPARENTLY DUE TO THE 200-MICROMETER UPPER LIMIT USED FOR THE PARTICLE DIAMETER IN THE QUICK CALCULATION, WHICH ALLOWED A SIGNIFICANT OVERFLOW OF PARTICLES FROM THE MESH. IN THE CONTAIN CALCULATIONS, A 5000-MICROMETER UPPER DIAMETER WAS USED. THE OVERFLOW OF PARTICLES FROM THE MESH IN THE QUICK CALCULATION EVIDENTLY HAD LITTLE EFFECT ON THE MASS CONCENTRATION (FIGURE AB-04).

   THE DIFFERENCE BETWEEN THE RESULTS FOR THE SETTLING DIAMETER IN THE TWO TYPES OF CONTAIN CALCULATIONS IS DUE PRIMARILY TO THE FACT THAT THE USE OF NON-STOKESIAN VELOCITIES IN THE QUICK TYPE OF MODELING REDUCES THE FALLOUT RATE OF LARGE PARTICLES SIGNIFICANTLY. THE VERY LARGE PARTICLES ARE, HOWEVER, RELATIVELY INEFFICIENT IN SWEEPING OUT SMALL PARTICLES, AND ONCE THEY DO FALL OUT, THE MASS CONCENTRATION IS RELATIVELY UNAFFECTED. THE DIFFERENCE BETWEEN THE MASS CONCENTRATIONS IN THE TWO TYPES OF CONTAIN CALCULATIONS IS DUE NOT SO MUCH TO STOKESIAN VERSUS NON-STOKESIAN VELOCITIES BUT TO OTHER MODELING DIFFERENCES.

   EXCEPT FOR THE DISCREPANCIES IN THE SETTLING DIAMETERS IN AB03, THE CAUSE OF WHICH HAS BEEN IDENTIFIED, THE COMPARISON BETWEEN THE TWO CODES IS GOOD TO EXCELLENT DEPENDING ON THE MODELS USED. THE FACT THAT THE DIFFERENT NUMERICAL SOLUTION SCHEMES IN CONTAIN AND QUICK PRODUCE ESSENTIALLY IDENTICAL RESULTS FOR THE SAME SET OF MODELS IS A STRONG INDICATION OF THE ADEQUACY OF THE COARSE-MESH (SECTIONAL) APPROACH USED IN CONTAIN. IT SHOULD BE NOTED THAT ABOUT ONE-HALF THE NUMBER OF SIZE CLASSES (SECTIONS) WERE USED IN THE CONTAIN CALCULATIONS AS COMPARED WITH THE QUICK CALCULATIONS, EVEN THOUGH A 5000-MICROMETER UPPER LIMIT WAS USED IN AB03 WITH CONTAIN.

9. COMMENTS: THE DETAILS OF THE PHYSICS MODELING IN QUICK WERE OBTAINED FROM REF 1, AND THE CHANGEOVER OF THE CONTAIN MODELS IS DOCUMENTED IN THE UPDATE CORRECTION SETS GIVEN WITH THE INPUT DATA SETS BELOW. NOTE THAT THE UPDATE CORRECTION SETS ALSO PROVIDE THE TIME-DEPENDENT TEMPERATURE GRADIENTS USED IN THE QUICK CALCULATIONS (A FEATURE NOT YET AVAILABLE IN CONTAIN) AND NONDEFAULT VALUES OF VARIOUS OTHER PARAMETERS.

   FROM THIS SET OF TESTS, IT HAS BEEN CONCLUDED THAT THE NUMERICAL SOLUTION SCHEME IN CONTAIN IS HIGHLY SATISFACTORY AND THAT THERE IS

NO COMPELLING REASON TO CHANGE THE CONTAIN PHYSICS MODELING. THE ADDITIONAL SHAPE FACTOR DEPENDENCE IN THE QUICK MODELS IS NOT ADEQUATELY JUSTIFIED AND SHOULD NOT BE IMPLEMENTED UNTIL PROPER JUSTIFICATION IS MADE. THE USE OF NON-STOKESIAN VELOCITIES IS DESIRABLE, BUT TYPICALLY, RELATIVELY LITTLE MASS OCCURS IN THE FORM OF LARGE PARTICLES. IN AB03, AT MOST A TEN PERCENT DIFFERENCE IN THE SUSPENDED MASS AND IN THE AERODYNAMIC MASS MEDIAN (NOT SETTLING) DIAMETER RESULTS FROM USE OF THE NON-STOKESIAN VELOCITIES. IN ADDITION, THE PARTICLE-SIZE RANGE REQUIRED TO TRACK THE LARGE PARTICLES MIGHT BE PROHIBITIVE BECAUSE OF STIFFNESS EFFECTS. CASES WHERE NON-STOKESIAN VELOCITIES ARE IMPORTANT CAN BE IDENTIFIED BY SIMPLY EXTENDING THE SIZE RANGE INTO THE APPROPRIATE REGIME. THE NON-STOKESIAN OPTION CAN BE IMPLEMENTED WHEN THE NEED BECOMES APPARENT.

10. SUGGESTIONS FOR ADDITIONAL TESTS: THE PRESENT TEST IS A TEST OF THE AGGLOMERATION AND DEPOSITION MODELING IN CONTAIN IN CASES WHERE TURBULENT AGGLOMERATION IS NOT IMPORTANT. TURBULENT AGGLOMERATION SHOULD BE TESTED BEFORE CONTAIN IS USED IN CASES WHERE IT IS IMPORTANT. IN ADDITION, THE ALGORITHM FOR CONDENSATION AND EVAPORATION OF WATER VAPOR ON AEROSOLS SHOULD BE TESTED.

REFERENCES:

1. H. Jordan, P. M. Schumacher, and J. A. Gieseke, QUICK Users' Manual, NUREG/CR-2105, BMI-2082, Battelle Columbus Laboratories, May 1981.

2. H. Jordan, P. M. Schumacher, and J. A. Gieseke, Comparison of QUICK Predictions with Results of Selected, Recent Aerosol Behavior Experiments, NUREG/CR-2922, BMI-2099, Battelle Columbus Laboratory, February, 1982, and H. Jordan, private communication.

3. R. K. Hilliard, J. D. McCormack, and A. K. Postma, Aerosol Behavior during Sodium Pool Fires in a Large Vessel: CSTF Tests AB-1 and AB-2, HEDL-TME-79-28, Hanford Engineering Development Laboratory, June, 1979.

4. J. D. McCormack, R. K. Hilliard, A. K. Postma, and R. K. Owen, "Aerosol Behavior during Sodium Spray Fires", Proceedings of the ANS-ENS International Meeting on Fast Reactor Safety Technology, Seattle, Washington, August, 1979, pp 823-831.

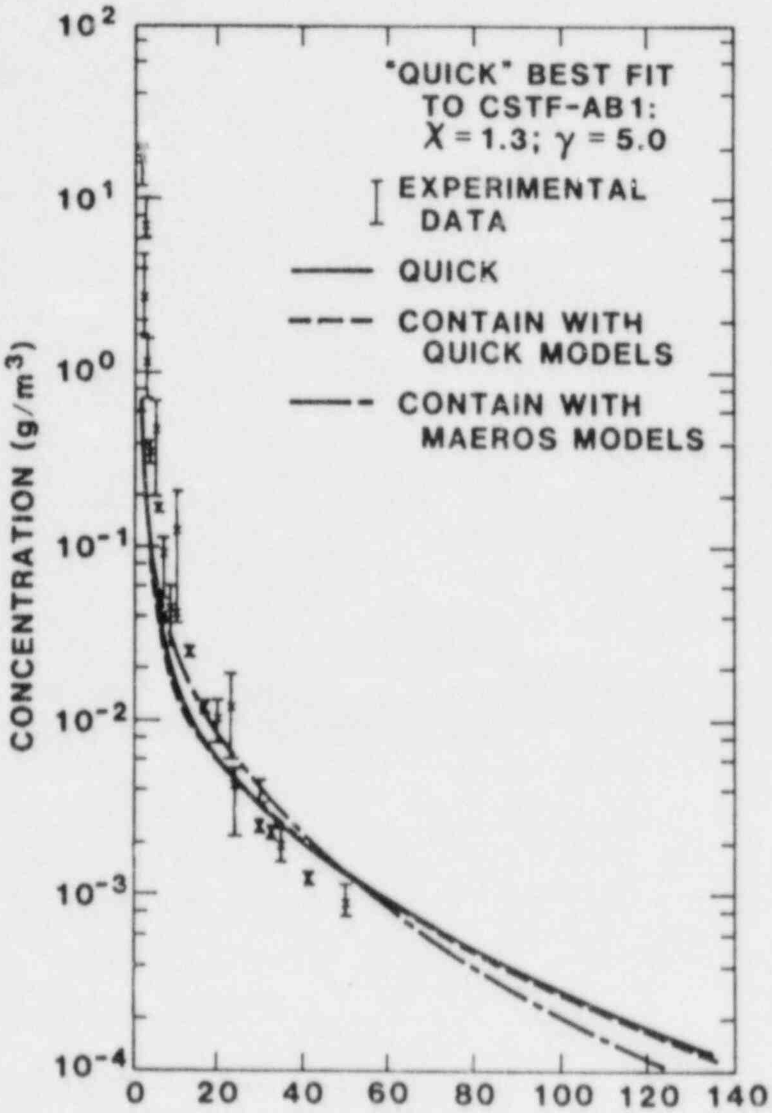

Figure AB-02 Comparison of QUICK calculations and two types of CONTAIN calculations of sodium oxide aerosol concentration for Experiment CSTF-AB1 (CONTAIN Test AB02).

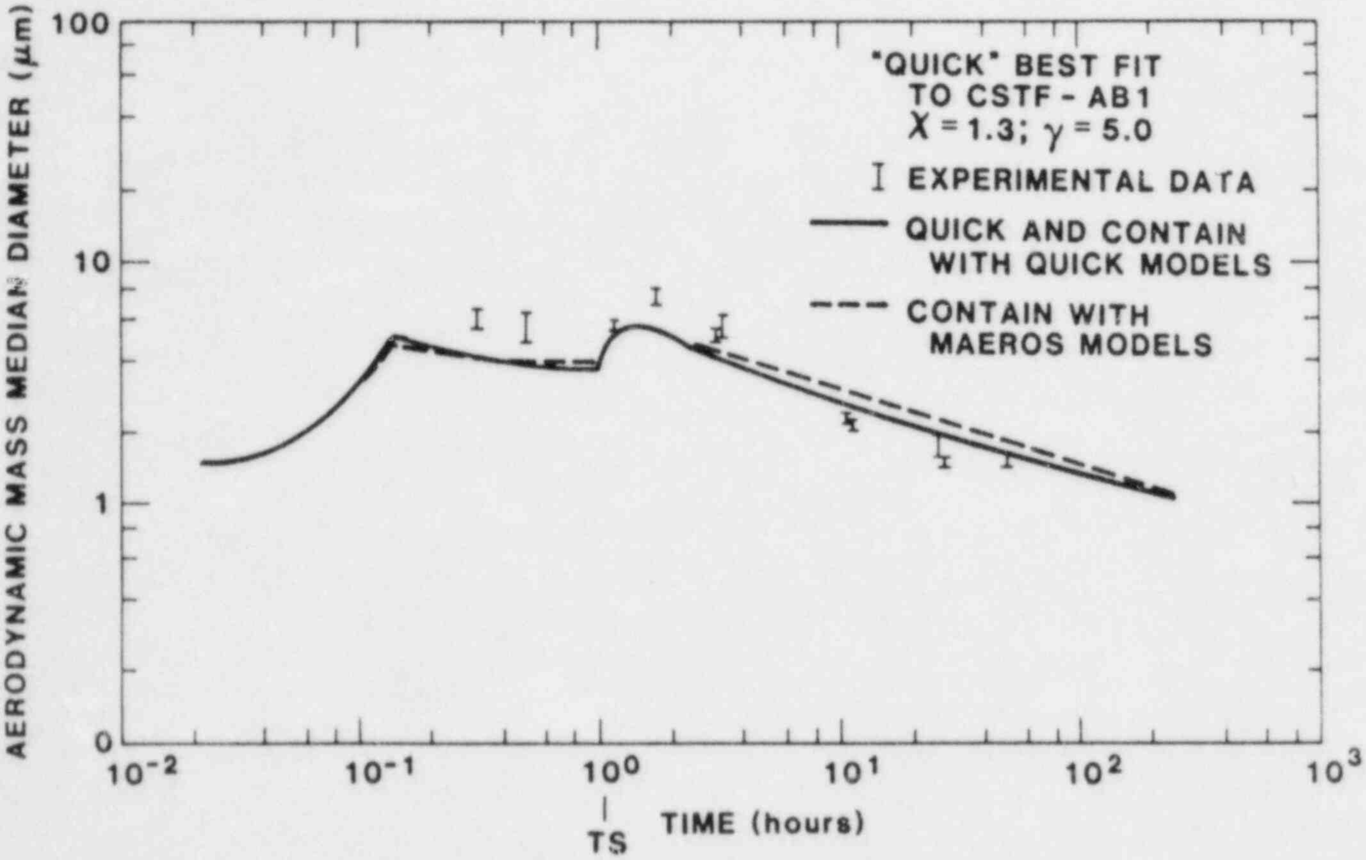

Figure AB-03 Mass aerodynamic median diameters from QUICK and CONTAIN calculations for Experiment CSTF-AB1 (CONTAIN Test AB02).

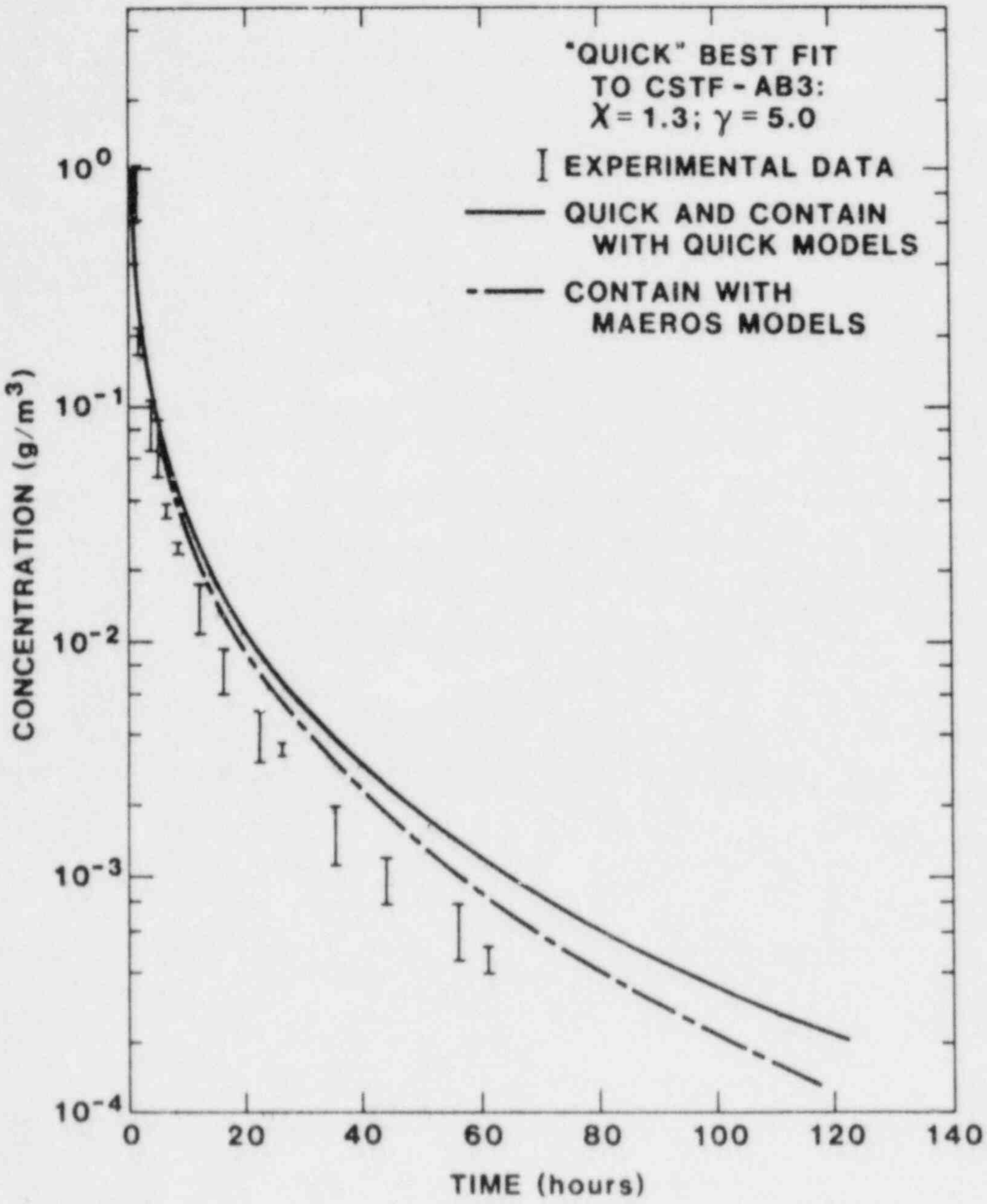

Figure AB-04 Comparison of QUICK and CONTAIN calculations of sodium oxide concentration for Experiment CSTF-AB3 (CONTAIN Test AB03).

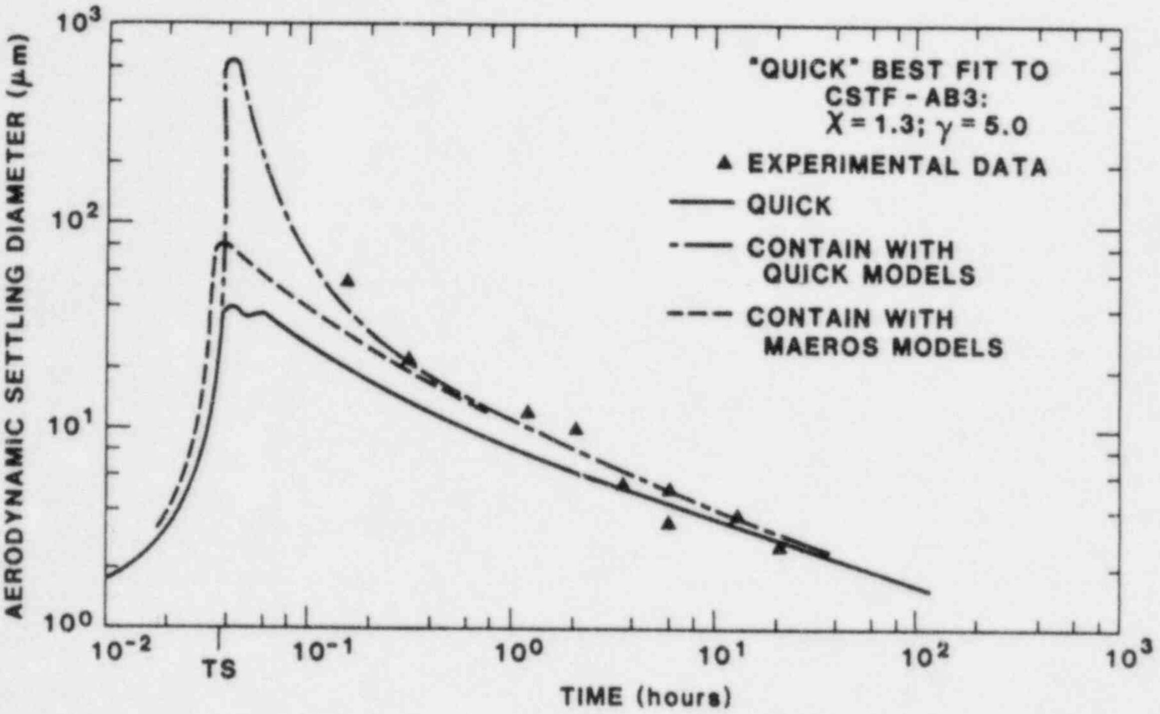

Figure AB-05 Aerodynamic settling diameters from QUICK and CONTAIN calculations for Experiment CSTF-AB3 (CONTAIN Test AB03).

SERIES AB TEST INPUT DATA SETS

The material that follows gives both the input data sets used for the AB tests and the CONTAIN coding updates necessary for these runs,

```
------------------------ AB01(ST) --------------------------------
*/ =================================================================
*/
*/ SOME PHYSICS MODELING PARAMETERS ARE SET HERE THROUGH CODE UPDATES
*/ FOR NSPP207 BEST FIT RUN B
*/
*D A-CHI.7
      CHI=1.5
*D A-GAMMA.7
      GAMMA=7.
*D A-RHODD.9
      RHO=8.30E3
*/
*/ END OF CODE UPDATES
*/
*/ ============================================================
&&
&& INPUT DATA SET FOR NSPP207 BEST FIT RUN B
&&
CONTROL = 9 1 1 2 2 1 20 2 0 0
MATERIAL
 COMPOUND N2 O2 NAL NAV NA2O PUO2
 FISSION DUMY1 DUMY2
TIMES 1000. 1548. 1000. 999. 12548. 10000. 9999. 122548. 1.
PRAER
FISSION
 0
 2
 DUMY1 DUMY2
 1.0E10 1.0E20
 0. 0.
 EOI
TITLE
 NSPP207 COMPARISON TEST

AEROSOL  1 0 0 0 0 1.01E5 0
 NA2O 1.05E-6 1.33
 PUO2 1.E-8 .401
CELL=1
CONTROL  = 20 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
GEOMETRY 38.3 5.49
ATMOS=2
 1.01E5 323.
 N2=.79    O2=.21
 AEROSOL=1
 NA2O= .1313
EOF
----------------------- END OF AB01 ---------------------------
```

```
---------------------------- AB02 ----------------------------------
*/ CODE UPDATES ARE REQUIRED TO RUN THIS COMPARISON TO THE QUICK CODE.
*/ THE FIRST BLOCK OF UPDATES BELOW SHOULD BE USED TO CONVERT THE
*/ CONTAIN MODELS TO THE QUICK MODELS.  THE SECOND BLOCK OF UPDATES
*/ SETS MODEL PARAMETERS WHICH CANNOT CURRENTLY BE SET THROUGH THE
*/ CONVENTIONAL CONTAIN INPUT.  THE CONVENTIONAL CONTAIN INPUT DATA
*/ SET FOLLOWS THE TWO UPDATE SETS.
*/===================================================================
*/
*IDENT QUPDAT
*/
*/ THE FOLLOWING UPDATES CONVERT THE CONTAIN MODELS TO THE QUICK
*/ MODELS
*/
*/ THE CHANGE FROM STOKES VELOCITIES TO NON-STOKES IS ACCOMPLISHED
*/ IN THE FOLLOWING BLOCK
*/
*D A-DEPOST.21
      CALL SETTLE(.5*D,VTERM,GAMMA(V),CHI(V),VISCOS,DENAIR,RHO,
     1 9.8,IFFFF)
*I A-DEPOST.30
      SUBROUTINE SETTLE(R,VEL,GAMMA,CHI,ETA,RHOG,RHOP,G,IFLAG)
      REAL LGRE,LGR2CF
      DIMENSION LGRE(52),LGR2CF(52)
      DATA LGR2CF/-.620,-.519,-.419,-.318,-.218,-.117,-.017,
     1.084,.185,.286,.387,.487,.591,.693,.795,
     1.898,1.002,1.107,1.213,1.321,1.430,1.541,1.654,
     11.769,1.886,2.006,2.128,2.252,2.378,2.506,2.636,
     12.768,2.902,3.038,3.175,3.314,3.455,3.598,3.743,
     13.890,4.039,4.191,4.345,4.502,4.661,4.823,4.987,
     15.154,5.323,5.495,5.671,5.850/
      LGRE=-2.
      DO 11 I=2,52
   11 LGRE(I)=LGRE(I-1)+.1
      X=10.666667*RHOG*RHOP*G*R*R*R*GAMMA
      X=X/(CHI*ETA*ETA)
      X=ALOG10(X)
      IF(X.LT.-.620) GO TO 1
      IF(X.GT.5.850) GO TO 2
      DO 22 I=1,52
      I1=I-1
      DIF=LGR2CF(I)-X
      ADIF=ABS(DIF)
      IF(ADIF.LT.1.E-4) GO TO 3
      IF(DIF.LT.0.) GO TO 22
      I2=I
      GO TO 10
   22 CONTINUE
   10 DELX=LGR2CF(I2)-LGR2CF(I1)
      F=(X-LGR2CF(I1))/DELX
      Y=LGRE(I1)+.1*F
      GO TO 20
    1 VEL=.22222222*RHOP*G*R*R/(ETA*CHI)
      RETURN
```

```
    2 IFLAG=1
      RETURN
    3 Y=LGRE(I1)
   20 Y=10**Y
      VEL=ETA*Y/(2.*R*RHOG*GAMMA)
      RETURN
      END
*/
*/ THE SHAPE FACTOR DEPENDENCE OF THE KNUDSEN NUMBER IS INSERTED HERE
*/
*I A-BETA.23
      AKX=AKX/GAMMA(V)
      AKY=AKY/GAMMA(U)
*I A-DEPOST.19
      AKN=AKN/GAMMA(V)
*/
*/ THE GRAVITATIONAL COLLISION KERNEL IS INTRODUCED HERE. NOTE
*/ LACK OF NON-STOKESIAN AND MEAN FREE PATH CORRECTIONS
*/
*D A-BETA.33,34
      VABDIF=.54444*ABS(RHOX*DX*DX/FCHIX-RHOY*DY*DY/FCHIY)/VISCOS
*/
*/ THE BROWNIAN MOTION KERNEL IS INTRODUCED HERE. NOTE ABSENCE OF
*/ MEAN FREE PATH CORRECTIONS
*/
*D A-BETA.49,50
      BETA=6.2832*(DIFX+DIFY)*DSUM
*/
*/ THE THERMOPHORESIS COEFFICIENT IS INTRODUCED HERE.
*/
*D A-DEPOST.23,24
      VTHRML=1.5*VISCOS*BMOBIL*(2.49*AKN+1.0)/(FCHI*DENAIR
     1 *(1.+3.*AKN)*(1.+2.*(2.49*AKN+1.)))*GAMMA(V)
*/
*/ END OF MODEL CONVERSION BLOCK
*/
*/ ===============================================================
*/
*IDENT PUPDAT
*/
*/ PHYSICS MODELING PARAMETERS ARE SET HERE
*/
*/
*/ THE FOLLOWING INTRODUCES A TIME-DEPENDENT WALL-GAS TEMPERATURE
*/ DIFFERENTIAL
*/
*I A-ACNTRL.23
      DIMENSION TDATA(20),DTDATA(20)
      DATA TDATA/
     1 0. ,60.,180.,300.,420.,
     1 540.,1140.,1860.,2220.,2580.,
     1 2940.,3300.,5100.,8700.,12300.,
     1 15900.,24900.,33900.,50400.,1.E7/
      DATA DTDATA/
```

```
     1 .3,19.,16.5,16.1,18.5,
     1 20.6,24.6,27.1,26.4,26.7,
     1 31.4,29.7,10.2,6.2,5.6,
     1 4.6,3.4,2.7,2.1,0./
*I A-ACNTRL.104
      DTWALL=0.
      IF(TIME.LT.TDATA(1).OR.TIME.GT.TDATA(19)) GO TO 202
      TMID=TIME+.5*DT
      DO 200 KT=1,19
      IF(TMID.LT.TDATA(KT)) GO TO 201
  200 CONTINUE
      GO TO 202
  201 DTWALL=(DTDATA(KT)*(TMID-TDATA(KT-1))-DTDATA(KT-1)*(TMID-
     1 TDATA(KT)))/(TDATA(KT)-TDATA(KT-1))
  202 DELTH=.015
      TGRADC=DTWALL/DELTH
      TGRADW=DTWALL/DELTH
      TGRADF=DTWALL/DELTH
*/
*/ THE FOLLOWING SETS VARIOUS OTHER PARAMETERS
*/
*D A-ACNTRL.106,108
      ACELOV=0.
      AWALOV=1.073
      AFLROV=.1035
*D A-CHI.7
      CHI=1.3
*D A-GAMMA.7
      GAMMA=5.
*D A-RHODD.9
      RHO=2.2450E3
*I A-COEF.23
      TURBDS=0.
      DELDIF=.0001
      TKGOP=1.
*/
*/ END OF AB02 UPDATE BLOCKS
*/
*/ ======================================================================
&&
&& INPUT DATA SET FOR AB02
&&
CONTROL = 9 1 2 7 2 1 20 3 0 0
MATERIAL
 COMPOUND N2 O2 H2 CO2 H2OL H2OV NAM NAV NAOH NA2O NA2O2 GRAPH
 FE
 FISSION DUMY1 DUMY2
TIMES 1000. 0. 20. 20. 500. 100. 100. 1000.
200. 800. 3600. 2000. 1000. 10000. 2000. 10000. 30000.
2000. 10000. 100000. 2000. 100000. 400000. 1.
PRFLOW
PRHEAT
PRAER
PRH-BURN
```

```
FLOWS
FISSION
 0
 2
 DUMY1 DUMY2
 1.0E10 1.0E20
 0. 0.
 EOI
TITLE
 AB1 (EXPERIMENT) COMPARISON TEST

 THERMAL
AEROSOL  1 .1E-6 500.E-6 0 0 0 0
 NA2O 1.E-6 .693
 NAOH 1.E-6 .693
H2OV 2.E-6 .5
CELL=1
CONTROL=20 0 0 0 0 0 0 0 0 0 0 0 1 7 0 0 0 0 0 0 0 0
GEOMETRY 850. 20.3
ATMOS=2
 1.212E5 338.15
 N2=.79    O2=.21
CONDENSE
 AEROSOL=1
  NA2O= .0001
 SOURCE=1
 NA2O=7 IFLAG=1
 T=0. 600. 1200. 1800. 2400. 3000. 3600.
 MASS=.03175 .01784 .01751 .01555 .0152 .0152 0.
 TEMP= 298. 298. 298.
 EOI
EOF
---------------------------- END OF AB02 ------------------------------

-------------------------------- AB03 ---------------------------------
*/ CODE UPDATES ARE REQUIRED TO RUN THIS COMPARISON TO THE QUICK CODE.
*/ THE FIRST BLOCK OF UPDATES BELOW SHOULD BE USED TO CONVERT THE
*/ CONTAIN MODELS TO THE QUICK MODELS.  THE SECOND BLOCK OF UPDATES
*/ SETS MODEL PARAMETERS WHICH CANNOT CURRENTLY BE SET THROUGH THE
*/ CONVENTIONAL CONTAIN INPUT.  THE CONVENTIONAL CONTAIN INPUT DATA
*/ SET FOLLOWS THE TWO UPDATE SETS.
*/====================================================================
*/
*IDENT QUPDAT
*/
*/ THE FOLLOWING UPDATES CONVERT THE CONTAIN MODELS TO THE QUICK
*/ MODELS
*/
*/ THE CHANGE FROM STOKES VELOCITIES TO NON-STOKES IS ACCOMPLISHED
*/ IN THE FOLLOWING BLOCK
*/
*D A-DEPOST.21
      CALL SETTLE(.5*D,VTERM,GAMMA(V),CHI(V),VISCOS,DENAIR,RHO,
     1 9.8,IFFFF)
```

```
*I A-DEPOST.30
      SUBROUTINE SETTLE(R,VEL,GAMMA,CHI,ETA,RHOG,RHOP,G,IFLAG)
      REAL LGRE,LGR2CF
      DIMENSION LGRE(52),LGR2CF(52)
      DATA LGR2CF/-.620,-.519,-.419,-.318,-.218,-.117,-.017,
     1.084,.185,.286,.387,.487,.591,.693,.795,
     1.898,1.002,1.107,1.213,1.321,1.430,1.541,1.654,
     11.769,1.886,2.006,2.128,2.252,2.378,2.506,2.636,
     12.768,2.902,3.038,3.175,3.314,3.455,3.598,3.743,
     13.890,4.039,4.191,4.345,4.502,4.661,4.823,4.987,
     15.154,5.323,5.495,5.671,5.850/
      LGRE=-2.
      DO 11 I=2,52
   11 LGRE(I)=LGRE(I-1)+.1
      X=10.666667*RHOG*RHOP*G*R*R*R*GAMMA
      X=X/(CHI*ETA*ETA)
      X=ALOG10(X)
      IF(X.LT.-.620) GO TO 1
      IF(X.GT.5.850) GO TO 2
      DO 22 I=1,52
      I1=I-1
      DIF=LGR2CF(I)-X
      ADIF=ABS(DIF)
      IF(ADIF.LT.1.E-4) GO TO 3
      IF(DIF.LT.0.) GO TO 22
      I2=I
      GO TO 10
   22 CONTINUE
   10 DELX=LGR2CF(I2)-LGR2CF(I1)
      F=(X-LGR2CF(I1))/DELX
      Y=LGRE(I1)+.1*F
      GO TO 20
    1 VEL=.22222222*RHOP*G*R*R/(ETA*CHI)
      RETURN
    2 IFLAG=1
      RETURN
    3 Y=LGRE(I1)
   20 Y=10**Y
      VEL=ETA*Y/(2.*R*RHOG*GAMMA)
      RETURN
      END
*/
*/ THE SHAPE FACTOR DEPENDENCE OF THE KNUDSEN NUMBER IS INSERTED HERE
*/
*I A-BETA.23
      AKX=AKX/GAMMA(V)
      AKY=AKY/GAMMA(U)
*I A-DEPOST.19
      AKN=AKN/GAMMA(V)
*/
*/ THE GRAVITATIONAL COLLISION KERNEL IS INTRODUCED HERE. NOTE
*/ LACK OF NON-STOKESIAN AND MEAN FREE PATH CORRECTIONS
*/
*D A-BETA.33,34
```

```
      VABDIF=.54444*ABS(RHOX*DX*DX/FCHIX-RHOY*DY*DY/FCHIY)/VISCOS
*/
*/ THE BROWNIAN MOTION KERNEL IS INTRODUCED HERE. NOTE ABSENCE OF
*/ MEAN FREE PATH CORRECTIONS
*/
*D A-BETA.49,50
      BETA=6.2832*(DIFX+DIFY)*DSUM
*/
*/ THE THERMOPHORESIS COEFFICIENT IS INTRODUCED HERE.
*/
*D A-DEPOST.23,24
      VTHRML=1.5*VISCOS*BMOBIL*(2.49*AKN+1.0)/(FCHI*DENAIR
     1 *(1.+3.*AKN)*(1.+2.*(2.49*AKN+1.)))*GAMMA(V)
*/
*/ END OF MODEL CONVERSION BLOCK
*/
*/ ================================================================
*/
*IDENT PAB-3
*/
*/ PHYSICS MODELING PARAMETERS ARE SET HERE
*/
*I A-ACNTRL.23
      DIMENSION TDATA(20),DTDATA(20)
      DATA TDATA/
     1 0.,20.,60.,100.,
     1 120.,140.,180.,240.,
     1 300.,360.,420.,480.,
     1 600.,720.,900.,1200./
      DATA DTDATA/
     1 0.,110.,390.,430.,
     1 445.,460.,323.,175.,
     1 122.,97.,76.,65.,
     1 50.,35.,23.,3./
*I A-ACNTRL.104
      DTWALL=0.
      IF(TIME.LT.TDATA(1).OR.TIME.GT.TDATA(16)) GO TO 202
      TMID=TIME+.5*DT
      DO 200 KT=1,16
      IF(TMID.LT.TDATA(KT)) GO TO 201
  200 CONTINUE
      GO TO 202
  201 DTWALL=(DTDATA(KT)*(TMID-TDATA(KT-1))-DTDATA(KT-1)*(TMID-
     1 TDATA(KT)))/(TDATA(KT)-TDATA(KT-1))
  202 DELTH=.02378
      TGRADC=DTWALL/DELTH
      TGRADW=DTWALL/DELTH
      TGRADF=DTWALL/DELTH
*D A-ACNTRL.106,108
      ACELOV=0.
      AWALOV=1.073
      AFLROV=.1035
*D A-CHI.7
      CHI=1.3
```

```
*D A-GAMMA.7
      GAMMA=5.
*D A-RHODD.9
      RHO=2.270E3
*I A-COEF.23
      TURBDS=0.
      DELDIF=.0001
      TKGOP=1.
*/
*/ END OF AB03 UPDATE BLOCKS
*/
*/ =================================================================
&&
&& INPUT DATA SET FOR AB-3
&&
CONTROL = 9 1 2 7 2 1 28 3 0 0
MATERIAL
 COMPOUND N2 O2 H2 CO2 H2OL H2OV NAL NAV NAOH NA2O NA2O2 GRAPH
 FE
 FISSION DUMY1 DUMY2
TIMES 1000. 0. 20. 20. 500. 100. 100. 1000.
200. 800. 3600. 2000. 1000. 10000. 2000. 10000. 30000.
2000. 10000. 100000. 2000. 100000. 400000. 1.
PRFLOW
PRHEAT
PRAER
PRH-BURN
FLOWS
FISSION
 0
 2
 DUMY1 DUMY2
 1.0E10 1.0E20
 . 0.
 EOI
TITLE
 AB3 (EXPERIMENT) COMPARISON TEST

 THERMAL
AEROSOL  1 .1E-6 5000.E-6 0 0 0 0
 NA2O 1.E-6 .385
 NAOH 1.E-6 .693
H2OV 2.E-6 .5
CELL=1
CONTROL=20 0 0 0 0 0 0 0 0 0 0 1 7 0 0 0 0 0 0 0 0
GEOMETRY 850. 20.3
ATMOS=2
 1.212E5 338.15
 N2=.79    O2=.21
CONDENSE
 AEROSOL=1
  NA2O= .0001
 SOURCE=1
 NA2O=3 IFLAG=1
```

```
 T=0. 140. 1.E7
 MASS=.5814 .0 .0
 TEMP= 298. 298. 298.
 EOI
EOF
--------------------------- END OF AB03 ------------------------------
```

3.7 INTEGRATED LWR SAMPLE PROBLEM

This test is unusual in that it is a large, integrated calculation involving many parts of the code. Although it is impossible to check the results against hand calculations, it is possible to examine the results qualitatively to determine if the general behavior is as it should be. Thus, it should be categorized as a qualitative test (TL2). There are no supporting calculations to supplement the Test Summary Report.

This test has been found to be an extremely useful tool for debugging new versions of the code, because so many of the atmosphere models are interacting with each other in the calculation.

CONTAIN TEST SUMMARY REPORT

1. IDENT NUMBER: ZT01 USER NAME: K. D. BERGERON

2. TEST LEVEL: TL2

3. TITLE OF TEST: LWR SAMPLE PROBLEM; TMLB' IN LARGE DRY CONTAINMENT

4. CODE VERSION (DATE): 501 (10/12/82); 120 (3/12/83)

5. ACTIVE MODULES OR OPTIONS: ATMOS. SOURCES, FISSION SOURCES, AEROSOL SOURCES, F.P. DECAY, CONDENSATION ON AEROSOLS AND STRUCTURES, FLOWS, RELEASE AND ACCEPTANCE OF F.P.S, H-BURN.

6. CONTAINMENT CONFIGURATION AND SOURCES: LARGE, DRY CONTAINMENT IN CELL 1, MODELED AFTER ZION (INCLUDING HEAT SINK). CONTAINMENT PARAMETERS (VOLUMES AND SIZES) WERE OBTAINED FROM MARCH INPUT DECKS AND HAVE NOT BEEN VERIFIED DIRECTLY. CELL 2 IS A LARGE VOLUME REPRESENTING THE OUTSIDE WORLD (AUX. BUILDINGS, ETC.) THE TMLB' SEQUENCE BEGINS WITH A STEAM BLOWDOWN 3300 SECONDS AFTER LOSS OF ON-SITE AND OFF-SITE POWER. LATE IN THE BLOWDOWN, HYDROGEN GAS IS RELEASED (AT 10300 S) BECAUSE THE CORE HAS BECOME UNCOVERED. VOLATILE FISSION PRODUCTS ALSO APPEAR (AT 11740 S); IN OUR CASE, THESE VOLATILE PRODUCTS ARE REPRESENTED BY I133. ALL THESE BLOWDOWN SOURCES ARE READ IN THROUGH TABLES. THE MARCH CODE WAS USED TO DETERMINE THE OVERALL TIMING OF THE BLOWDOWN, THOUGH THE STEAM PROFILE USED IS SLIGHTLY DIFFERENT FROM NOMINAL MARCH RUNS.

   THE BLOWDOWN IS OVER AROUND 9000 S. VESSEL FAILURE OCCURS AT 14500 S, RESULTING FIRST IN ADDITIONAL WATER SOURCES (THIS IS THE ACCUMULATOR WATER RELEASE) AND RELEASE OF ADDITIONAL HYDROGEN (ASSUMED STORED UP IN THE PRIMARY VESSEL). THERE THEN FOLLOWS A LONG PERIOD IN WHICH THE CORE INTERACTS WITH THE CONCRETE IN A DRY CAVITY. THIS RESULTS IN THE GENERATION OF MUCH CO, CO2, H2, AND H20 AT THE MELT TEMPERATURE (GAS BUBBLE THROUGH THE MOLTEN LAYER) AND OF AEROSOLS, WHICH ARE MODELED AS CONCRETE. FISSION PRODUCTS ARE GENERATED SIMULTANEOUSLY AND ASSOCIATE WITH THE CONCRETE AEROSOL. THESE ARE TE132 AND I133. THE I133 DECAYS TO XE133, WHICH IS RELEASED TO THE GAS. THE GAS GENERATION RATES WERE OBTAINED FROM THE CORCON SAMPLE PROBLEM. THE AEROSOL GENERATION RATE WAS BASED ON THE SANDIA INTERIM SOURCE-TERM CORRELATION--SEE MEMO BY J. BROCKMANN TO D. POWERS, APRIL 5, 1982 FOR HOW THIS IS

DONE. EARLY FISSION-PRODUCT SOURCES WERE BASED ON INPUT FROM A. R. TAIG, WHO USED WASH 1400 AS A STARTING POINT. (NOTE, HOWEVER, THAT THE PRESENT PROBLEM USES ONLY SAMPLE FISSION PRODUCTS AND IS EXTREMELY SIMPLISTIC.) LATE FISSION-PRODUCT SOURCES ARE BASED ON BROCKMANN'S MEMO, WHICH ALSO USES WASH 1400.

7. TEST: CHECK OPERATION OF ALL FEATURES OF THE CODE. VERIFY THAT ORDER OF MAGNITUDES ARE CORRECT (QUALITATIVE CHECKS).

8. RESULTS OF TEST: NUMEROUS BUGS WERE IDENTIFIED. MANY HAVE NOW BEEN FIXED. WITH THE UPDATE CORRECTIONS, WHICH HAVE BEEN INCLUDED IN SUBSEQUENT VERSIONS, THE JOB RUNS WITHOUT PROBLEMS ON VERSION 501. THE CORRECTIONS NEEDED ARE: (1) TO MAKE THE FISSION SOURCES WORK PROPERLY, AND (2) TO ALLOW FISSION PRODUCTS TO REMAIN ON AEROSOL HOSTS AS THEY PASS THROUGH A FLOW PATH. A FEW OTHER IDIOSYNCRACIES WERE FOUND WHICH COULD BE CORRECTED THROUGH THE INPUT. FOR EXAMPLE, WITH TOO SMALL AN UPPER LIMIT ON THE AEROSOL SIZE RANGE, THERE WAS TOO MUCH MATERIAL IN THE LAST BIN AND A SPURIOUS RUNAWAY PROBLEM OCCURRED, DEPLETING AEROSOL MASS TOO RAPIDLY AND GENERATING A TWO-PEAKED DISTRIBUTION.

   FIGURES ZT-01, -02, AND -03 DISPLAY SEVERAL KEY PARAMETERS FROM THE CONTAIN CALCULATIONS. FIGURE ZT-01 SHOWS THE PRESSURE IN CELL 1. THE TWO PRESSURE PEAKS CORRESPOND TO THE PRIMARY SYSTEM BLOWDOWN AND THE VESSEL FAILURE, RESPECTIVELY. FIGURE ZT-02 PRESENTS THE HYDROGEN MOLAR PERCENTAGE AS A FUNCTION OF TIME. THE LAST FIGURE GIVES THE AEROSOL CONCENTRATION VERSUS TIME IN CELL 2.

9. COMMENTS: ACTUAL RUNNING TIME WAS 38 SECONDS ON THE CRAY (CONTAIN VERSION 501). THIS WAS FOR A REAL TIME OF 77,000 S, AND IT INCLUDES PLOT TIME. (AEROSOL COEFFICIENTS WERE NOT RECALCULATED IN THIS RUN. IF THEY WERE, THERE WOULD BE AN ADDITIONAL 82-S CHARGE FOR VERSION 501.)

10. SUGGESTIONS FOR ADDITIONAL TESTS: PARAMETER-SENSITIVITY TESTS. COMPARISON WITH MARCH.

```
=================================================================
1.  PROBLEM:  ID NO.ZT01-01        2.  LEVEL:  PL3      3.  RESOLVED?  YES
4.  DESCRIPTION:  FISSION SOURCE OPTION DOES NOT WORK.  ALSO, IT STEPS
    ON FLOWS CALCULATION.  THE ERROR IS DUE TO AN UNDEFINED POINTER, LCFN.
    AN UPDATE WHICH CORRECTS THE PROBLEM HAS BEEN CHECKED OUT.
5.  DATE PROBLEM RESOLVED:  10/82
=================================================================
=================================================================
1.  PROBLEM:  ID NO.ZT01-02        2.  LEVEL:  PL3      3.  RESOLVED?  YES
4.  DESCRIPTION:  AEROSOL HOSTS LOSE THEIR ASSOCIATED FISSION PRODUCTS ON
    PASSSING THROUGH A FLOW PATH.  GAS HOSTS DO OK.  AN UPDATE TO FLWMA
    HAS BEEN WRITTEN THAT CORRECTS THE PROBLEM.
5.  DATE PROBLEM RESOLVED:  10/82
=================================================================
===================================================================
1.  PROBLEM:  ID NO.ZT01-03        2.  LEVEL:  PL1      3.  RESOLVED?  YES
4.  DESCRIPTION:  IT IS INCONVENIENT TO HAVE TO CHANGE INPUT DATASETS
    WHEN YOU CHANGE COMPUTERS. THE CRAY USES SCM, AND THE CDC USES LCM.
5.  DATE PROBLEM RESOLVED:  2/83.  VERSION 120 DOES NOT REQUIRE EITHER
===================================================================
```

1. PROBLEM: ID NO.ZT01-04 2. LEVEL: PL2 OR 3 3. RESOLVED? YES
4. DESCRIPTION: LARGE TEMPERATURE OSCILLATIONS IN STRUCTURE SURFACES. A PROBLEM IN NUMERICS THAT SEEMS TO BE LESS SEVERE WHEN DEFAULT AEROSOL COEFS ARE USED.
5. DATE PROBLEM RESOLVED: 2/83. CELL TIME STEP WAS TOO LONG FOR STABILITY OF HEAT-TRANSFER ALGORITHM

===

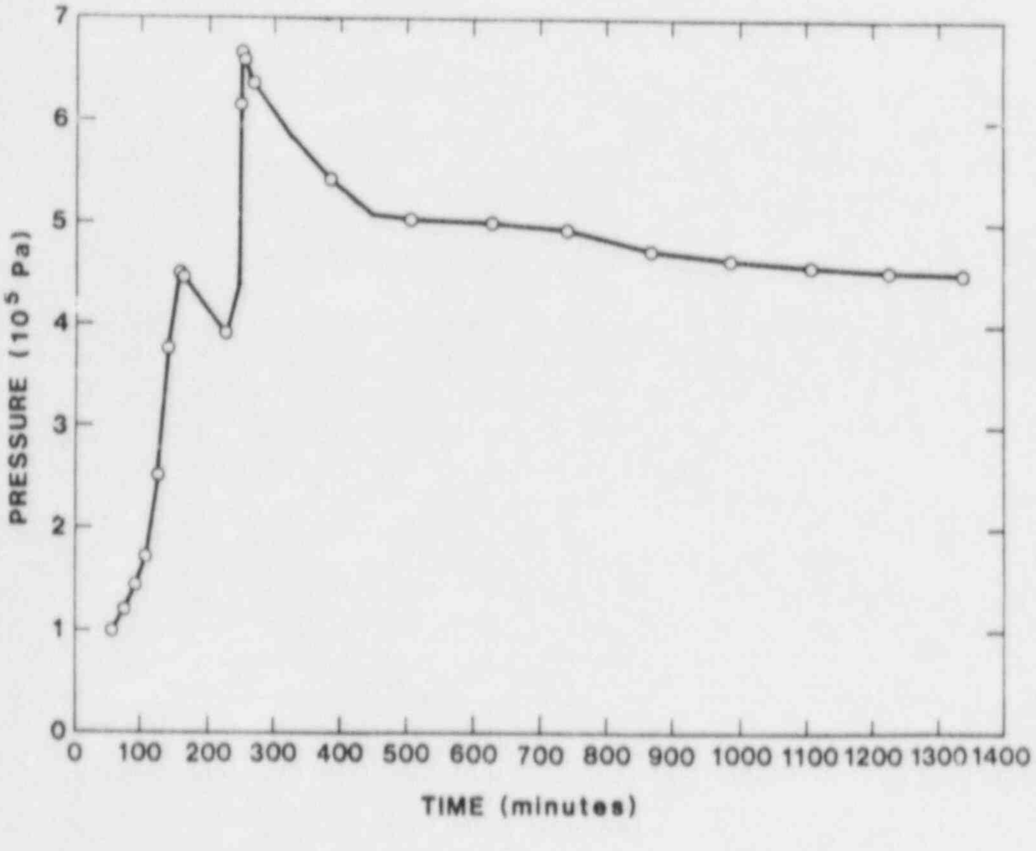

Figure ZT-01 Pressure in Cell 1: First peak is the blowdown in TMLB' sequence; second peak is vessel failure and accumulator discharge.

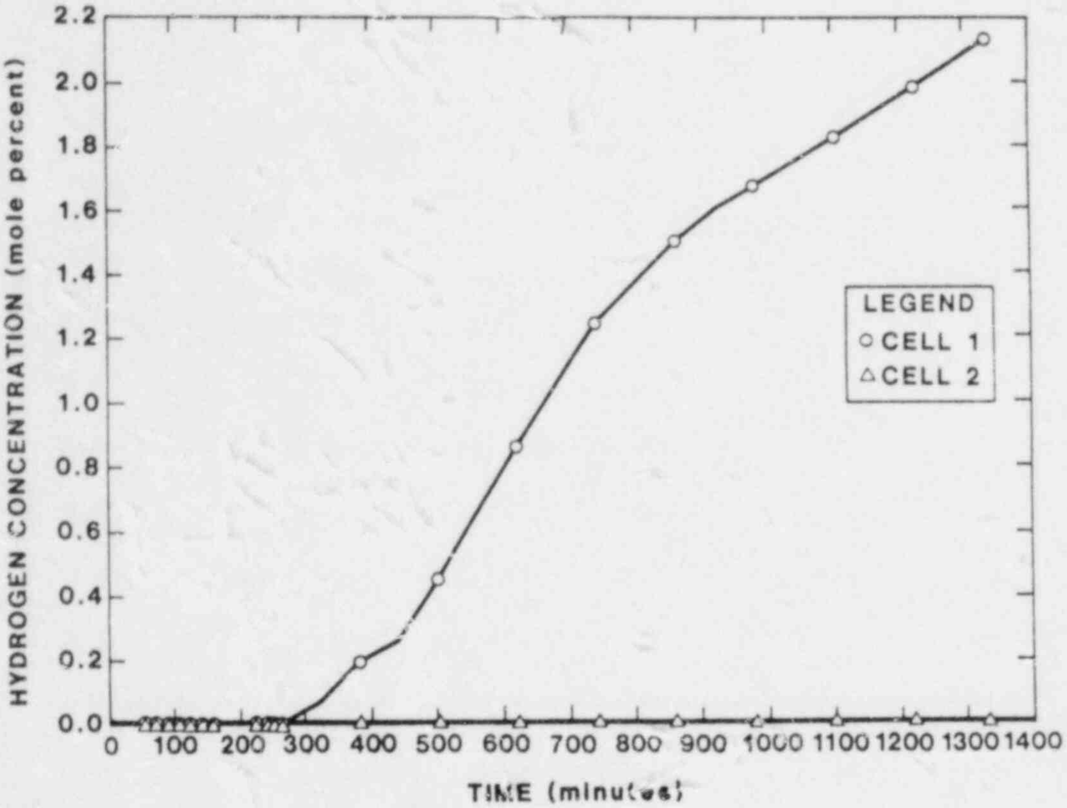

Figure ZT-02 Hydrogen concentration: Early hydrogen release before vessel failure is not visible; most of later hydrogen comes from core-concrete interaction.

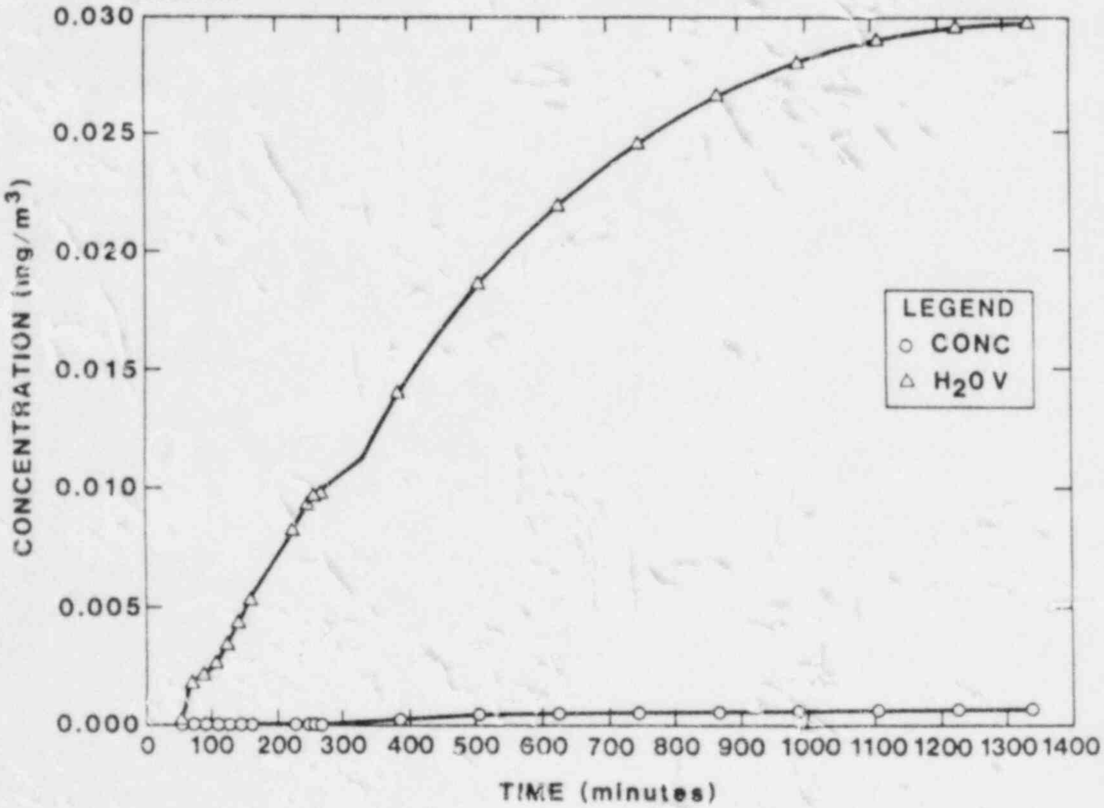

Figure ZT-03 Aerosol concentration in Cell 2: Cell 2 has very large volume and is intended to model small leak from containment to unsealed environment; consequently, aerosol flow is very small.

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4.0 FUTURE TESTING AREAS

Although significant progress has been made in testing CONTAIN, the testing program is by no means complete. As noted earlier, a program such as this is essentially impossible to complete. Certainly, the testing must continue as long as the code is under development.

Several areas for future test efforts have been identified. These areas are noted in the list below. Additional areas for testing will very likely be identified as the code undergoes development and testing progresses.

Two-Phase Atmosphere Thermodynamics (Water vapor or sodium vapor in a noncondensible gas atmosphere)
- Condensation of different vapors in different cells

Intercell Gas Flow
- Gas flow through many cells in series and in closed loops
- Gas flow through parallel flow paths

Surface Condensation
- Condensation of sodium vapor and related heat transfer

Aerosol Behavior
- Test turbulent-agglomeration models
- Condensation and evaporation of vapors on aerosols

Fission-Product Intercell Transport
- Transport into and through several cells in series
- Transport through parallel flow paths
- Check adequacy of host-material approach for treating fission-product movement and redistribution

Fission-Product Heating
- Atmosphere heating
- Pool heating
- Check adequacy for LWRs
- Check adequacy for LMFBRs

Sodium-Vapor Chemistry
- Atmosphere chemistry involving both H_2O and O_2 simultaneously

Sodium-Pool Fires
- Comprehensive comparison with state-of-the-art codes and with well characterized and well described experiments

Pool Heat Transfer
- Pool-to-structure heat transfer
- Pool interlayer heat transfer
- Pool-to-atmosphere heat transfer

Debris-Bed Dryout

Water Migration in Concrete
- Comparison with other codes and with experiments
- Checks of adequacy for channeling released water to adjacent cells

Sodium/Concrete Interactions

Debris/Concrete Interactions

Engineered Systems
- Containment Spray
- Liner failures
- Equipment modeling (pumps, valves, pipes, filters, supplies, etc.)
- Ice condenser systems
- Auxiliary cooling systems
- Fan coolers

Integrated LWR Test
- Comprehensive parametric and sensitivity studies
- Comparisons with other codes such as MARCH

Integrated LMFBR Test
- Perform integrated LMFBR tests
- Comprehensive parametric and sensitivity studies
- Comparisons with other codes such as CACECO

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