ANALYTICAL VALIDATION OF THE CACECO CONTAINMENT ANALYSIS CODE

Hanford Engineering Development Laboratory

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ANALYTICAL VALIDATION OF THE
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R. D. Peak

ABSTRACT

The CACECO containment analysis code was developed to predict the thermodynamic responses of LMFBF containment facilities to a variety of accidents. The code is included in the National Energy Software Center Library at Argonne National Laboratory as program No. 762.

This report covers the verification of the CACECO code by problems that can be solved by hand calculations or by reference to textbook and literature examples. The verification concentrates on the accuracy of the material and energy balances maintained by the code and on the independence of the four cells analyzed by the code so that the user can be assured that the code analyses are numerically correct and independent of the organization of the input data submitted to the code.

1

1

CONTENTS

	<u>Page</u>
Abstract	iii
Figures	vii
Tables	ix
1.0 SUMMARY	1
2.0 INTRODUCTION	3
3.0 DEBUG CASE DESCRIPTIONS MASS AND ENERGY DIFFERENTIAL EQUATIONS FOR ONE CELL	5
3.1 DEBUG CASES 1 TO 4, SODIUM SPRAYS AND SPACE COOLER OPERATION	10
3.1.1 Spray Hot Sodium into 100% Nitrogen	10
3.1.2 Spray Hot Sodium into 97.8% Nitrogen-2.2% Oxygen	15
3.1.3 Operate a Space Cooler to Cool a Cell	20
3.1.4 Cell Independence	22
3.2 DEBUG CASES 5 TO 8, SODIUM SPRAY AND SPILL AND AIR INJECTION	26
3.2.1 Spray Hot Sodium into 98.9% Nitrogen-1.1% Oxygen	27
3.2.2 Spill Hot Sodium into Cell with 97.8% Nitrogen- 2.2% Oxygen	31
3.2.3 Inject Cold Air into 96.7% Nitrogen-3.3% Oxygen	35
3.2.4 Cell Independence	39
3.3 DEBUG CASE 9, HEAT CONDUCTION IN PLANAR, CYLINDRICAL AND SPHERICAL HEAT STRUCTURES	44
3.4 DEBUG CASE 10, HEAT CONDUCTION IN SODIUM POOLS AND ANALYSES WITH RADIATION HEAT TRANSFER	68
3.5 DEBUG CASES 11 AND 12, RADIATION HEAT TRANSFER	95
3.6 DEBUG CASES 13, 14 AND 15, CONCRETE HEAT STRUCTURES	108

CONTENTS (Cont'd)

	<u>Page</u>
3.7 DEBUG CASES 16 TO 19, FISSION PRODUCT HEATING AND SPACE COOLER OPERATION	136
3.7.1 Fission Products Heat 96.7% Nitrogen-3.3% Oxygen Atmosphere	140
3.7.2 Fission Products Heat 6,880-lb Water Pool	141
3.7.3 Fission Products Heat 6,880-lb Sodium Pool	142
3.7.4 Fission-Product Heating Controlled by Space Cooler	143
3.7.5 Cell Independence	146
3.8 DEBUG CASES 20 TO 31, LEAKAGE CALCULATIONS CELL-TO-CELL	148
3.8.1 Leakage Calculations	150
3.8.2 Leakage of CO ₂ , N ₂ , O ₂ and H ₂ O	154
3.8.3 Leakage of H ₂ , N ₂ and Na	158
3.8.4 Cell Independence	160
3.9 DEBUG CASES 32, 33 AND 34, LEAKAGE CALCULATIONS TO CHECK ENERGY FUNCTIONS AND LEAKAGE CELL-TO-OUTSIDE	163
3.9.1 Thermodynamic Analysis	164
3.9.2 CACECO Check	166
3.10 DEBUG CASES 35 AND 36, SODIUM RECYCLE	170
4.0 REFERENCES	174
APPENDIX A Property Data Used Inside the CACECO Code	A-1
APPENDIX B CACECO Code Input Data (Microfiche) Card Pocket on Inside Back Cover	B-1

FIGURES

<u>Figure</u>		<u>Page</u>
3.1	Sodium Spray History for Cell A of Debug Case 5	28
3.2	Sodium Spill History for Cell B of Debug Case 5	33
3.3	Air Injection History for Cell C of Debug Case 5	36
3.4	Comparison of CACECO and Analytical Temperatures In the Slab: Structures 1 and 2	53
3.5	Comparison of CACECO and Analytical Temperatures In the Slab: Structures 3 and 4	54
3.6	Comparison of CACECO and Analytical Temperatures In the Slab: Structures 5 and 6	55
3.7	Comparison of CACECO and Analytical Temperatures In the Slab: Structures 7 and 8	56
3.8	Comparison of CACECO and Analytical Temperatures In the Slab: Structures 9 and 10	57
3.9	Comparison of CACECO and Analytical Temperatures In the Cylinder: Structures 11 and 12	58
3.10	Comparison of CACECO and Analytical Temperatures In the Cylinder: Structures 13 and 14	59
3.11	Comparison of CACECO and Analytical Temperatures In the Sphere: Structures 15 and 16	60
3.12	Comparison of CACECO and Analytical Temperatures In the Sphere: Structures 17 and 18	61
3.13	Heat Structures for Debug Case 10	72
3.14	Comparison of CACECO and Analytical Temperatures for the Well-Stirred Fluid	77
3.15	Comparison of CACECO and Analytical Temperatures In the Slab: Structure 1 (in contact with sodium) and Structure 7 (in contact with water pool)	79

FIGURES (Cont'd)

<u>Figure</u>		<u>Page</u>
3.16	Comparison of CACECO and Published Temperatures For the Slab: Structure 3 (sodium pool of Cell B) and Structure 4 (steel slab)	88
3.17	Comparison of CACECO and Analytical Temperatures In the Slab: Structure 4 (concrete slab), Structure 5 (sodium slab), Structure 6 (steel slab) and Structure 10 (Cell C sodium pool)	94
3.18	Six-Surface Example of Radiation Heat Transfer by Clark, Lammers, Kreplin and Korybalski	98
3.19	Limestone Concrete Properties Used in Debug Cases 13 Through 15	110
3.20	Comparison of CACECO and Analytical Temperatures In the Slab: Structure 1 (water release) and Structure 4 (carbon dioxide release)	113
3.21	Comparison of CACECO and Analytical Temperatures In the Cylinder: Structure 2 (water release) and Structure 5 (carbon dioxide release)	114
3.22	Comparison of CACECO and Analytical Temperatures In the Sphere: Structure 3 (water release) and Structure 6 (carbon dioxide release)	115
3.23	CACECO Results for Debug Case 35 with 10,000 lb/hr Spray of Sodium	172
3.24	CACECO Results for Debug Case 35 with 10,000 lb/hr Spill of Sodium	173

TABLES

<u>Table</u>	<u>Page</u>
3.1 Debug Cases 1 Through 4	25
3.2 Debug Cases 5 Through 8	43
3.3 Simulation Parameters Checked by Case 9	47
3.4 Code Parameters Checked by Case 9	48
3.5 Volumetric Heating Parameters of Case 9	50
3.6 Heat-Transfer Coefficient Check of Case 9	52
3.7 Check Case 9 Sums of Heat-Transfer Rates	63
3.8 Check Case 9 Energy Transfers	64
3.9 Check Case 9 Sums of Energy Transfers	66
3.10 Case 9 Cell Atmospheres	67
3.11 Simulation Parameters Checked by Case 10	70
3.12 Code Parameters Checked by Case 10	71
3.13 CACECO Check of Hot Pool Cooled by Cold Floor	75
3.14 CACECO Check of Hot Pool Cooled by Radiation	84
3.15 Cell C Pool Cooling Parameters	90
3.16 CACECO Check of Hot Pool Cooled by Three Floors	92
3.17 Internal Radiation View Factors for Six-Surface Example	100
3.18 Internal Total Interchange Areas for Six-Surface Example	101
3.19 External Total Interchange Areas for Both Examples	102
3.20 Check Case 11 Temperatures	104
3.21 Check Case 11 Heat Exchanges	105
3.22 Check Case 12 Temperatures	107

TABLES (Cont'd)

<u>Table</u>	<u>Page</u>
3.23 Check Case 13 Material Releases and Energy Transfers	119
3.24 Results of Cases 13, 14 and 15	131
3.25 Check Cases 13, 14 and 15 Sodium Pool Responses	132
3.26 Debug Cases 16 Through 19	147
3.27 Plan of Debug Cases 20 to 31	149
3.28 Conditions for CO ₂ , N ₂ , O ₂ and H ₂ O Leakage Check	157
3.29 Conditions for H ₂ , N ₂ and Na Leakage Check	161
3.30 Debug Cases 20 Through 31	162
3.31 Plan of Debug Cases 32, 33 and 34	163
3.32 Debug Cases 32, 33 and 34	168

ANALYTICAL VALIDATION OF THE
CACECO CONTAINMENT ANALYSIS CODE (WXYAEB)

1.0 SUMMARY

The CACECO containment analysis code was developed to predict the thermodynamic responses of LMFBR secondary containment to a variety of facility accidents such as: (a) sodium leakage as spray and spill, (b) air injection, (c) decay-heat release, and (d) space-cooler operation. The prediction is based on numerical solutions to the mass and energy differential equations for each of the four cells treated by the code. The code has been included in the National Energy Software Center Library at Argonne National Laboratory. It is described in computer program Abstract 762.

This report covers the verification of the CACECO code by problems that can be solved by (a) hand calculations or by reference to (b) textbook examples and (c) literature examples. The many problems treated in this verification suggest the large variety of situations that can be analyzed by the code. Generally the verification had the following plan: (a) invent simple problems in order to check one code feature at a time, (b) check all possibilities of this feature, and (c) combine features as required to check the next feature. The verification used 36 cases, which are called Debug Cases because they were invented to debug the code. That is, the cases were invented to prove to the code writer, as well as to the user, that the code operates as described in the Users' Guide.

This report has been organized with the assumption that the reader will start at the beginning and progress on through; thus, a topic discussed at the beginning is not discussed again. For example, Section 3.1 details the calculation of initial conditions and the operation of sodium sprays from the input data of Cards 2 through 9 and Card Series 401 through 701; Section 3.10 assumes that initial conditions and sodium sprays are understood and

details the calculation of sodium recycle from the input data of Card 2100. The report concentrates on the accuracy of material and energy balances and on the independence of the four cells analyzed by the code so that the user can be assured that the code analyses are correct and independent of the cell.

The 36 Debug Cases described in this verification report take 263 system seconds to run on the Control Data Corporation Cyber-74 computer at a cost of about \$26. These cases cover all input data cards except Card Series 2401 (which describes sodium-concrete reactions), and all phenomenon except the sodium-concrete reaction and the hydrogen-oxygen reaction. These two reactions were skipped in this verification because there are important experimental investigations presently underway on these topics; thus, the code algorithms on these reactions must be considered temporary.

2.0 INTRODUCTION

The CACECO code was developed to predict the thermodynamic responses of LMFBR secondary containment to a variety of facility accidents such as: (a) sodium leakage as spray and spill, (b) air injection, (c) decay-heat release, and (d) space-cooler operation. The code treats each vessel, cavity, vault, cell, pipeway, or building as an analysis cell and can analyze the conditions in one cell, two cells, or in three or four cells according to the needs of the accident scenario. These analysis cells are called Cell A, Cell B, Cell C, and Cell D. There is little specialization in the code; each cell has the same provisions as Cell A and can be used to obtain the same results. The code calculates cell conditions (such as temperature and pressure from mass and energy balances that include chemical reactions, carbon-dioxide and water-vapor releases upon heating of concrete, decay power, atmosphere leakages, sodium transfers between cells, etc.,) so as to accommodate the various phenomena of accident scenarios for LMFBR facilities.

This report covers the verification of the CACECO code by problems that can be solved by (a) hand calculations or by comparison with (b) textbook examples and (c) literature examples. Many of these problems were invented in order to debug the code as it was being developed and were thereby called Debug Cases because they were to prove to the code author that the code operated as described in the Users' Guide.⁽¹⁾ Generally the verification had the following plan: (a) begin with a problem which checks one code feature, (b) check all possibilities of this feature, (c) progress to check another feature, and (d) combine verified features as required to check the next feature. This verification used 36 cases to check the code. The many problems of these cases suggest the large variety of situations that can be analyzed by the code.

An important concern to the code author was verification of the CACECO capability that each cell has the same provisions as Cell A and could be

used to obtain the same results. This code capability can be expressed in a variety of ways:

1. CACECO analyses are not dependent upon the cell used, and Cells A, B, C and D are equivalent.
2. CACECO analyses are not dependent upon the organization of the input data.
3. The cells are independent of one another.

This code capability was verified by using different volumes and initial conditions in the active cells of each case and then rotating these volumes and conditions around the cells in a sequence of cases.

The CACECO code verification is proven by an exact correspondence between the numbers in this report and the numbers in the computer printout. The report describes the calculation or justification of these numbers. The calculations use the property data listed in Appendix A. The computer input data* are listed in Appendix B, and the author assumes that the reader has run the Debug Cases of interest and has the computer printout at hand during his review of this report. The exact correspondence is shown by underlining the number in this report and citing in the margin either: (a) the Appendix B page number for input data or (b) the case and computer printout page number for output results. This citation facilitates the reader's check of the numbers of interest.

* A card copy of these input data is available from the author.

3.0 DEBUG CASE DESCRIPTIONS

The main purpose of these debug problems was to prove to the code author and to interested code users that the CACECO code would provide acceptable predictions of the containment responses to a variety of facility accidents. These problems, hereafter called cases, were organized on the basis of checking the code use of input data because the input data provide the descriptive model of the containment situation being analyzed. For example, Debug Case 1 checks input Cards 2 and 3, which describe a situation wherein 51 lb of hot sodium are sprayed into a 1001-ft³ cell filled with 100% nitrogen. Debug Case 2 checks input Cards 2 and 3, which describe a similar situation wherein 543 lb of sodium are sprayed into a 2020-ft³ cell filled with 2.2% oxygen and 97.8% nitrogen. Finally, Debug Case 3 checks input Cards 2 and 1700, which describe a third situation having a space cooler operating in a 4444-ft³ cell filled with air. In general, these debug cases will treat all of the input data cards that are described in the CACECO Users' Guide.

Each case is described in terms of the mathematical model that it solves.* The principle mathematical models are represented by the five differential equations that express the mass and energy balances of each cell analyzed by the code. Since there are four cells analyzed by the code, there are four sets of these five equations. Each set of these differential equations includes three equations which describe the mass balances of the atmosphere, sodium pool and water pool and two equations which describe the energy balances of the atmosphere and pool. One set of these five equations is listed in the following pages. The nomenclature of these equations is informal. Usually the letter denoting each variable is the first alphabetic letter of the phenomenological name of that variable. For example, M represents Mass, and I represents Input data. Each case will be presented in terms of checking a portion of one or more of these differential equations.

ATMOSPHERE MASS DIFFERENTIAL EQUATION

$$\frac{d}{dt} M_a = \text{atmosphere mass change in Cell J} \quad (3.0.1)$$

$$= I_{Na} + I_{N_2} + O_2$$

Input tables for sodium spray and gas injection

$$+ \sum_I L_{IJ} - \sum_K L_{JK}$$

Leakage from Cell I and to Cell K

$$- R_{Na + CO_2} - R_{Na + O_2} - R_{Na + H_2O}$$

Chemical reactions of sodium with carbon dioxide, oxygen, and water vapor

$$+ R_C + R_{Na_2O} + R_{H_2}$$

Chemical reaction products of carbon, sodium oxide, and hydrogen

$$- R_{Na + H_2} - R_{Na_2O + H_2O}$$

Chemical reaction of sodium with hydrogen and of sodium oxide with water vapor

$$- R_{H_2 + O_2} + R_{H_2O}$$

Chemical reaction of hydrogen and oxygen to make water vapor.

$$+ R_{NaH} + R_{NaOH}$$

Chemical reaction products of sodium hydride and sodium hydroxide

$$+ \sum_N R_{CO_2} + \sum_N R_{H_2O}$$

Concrete releases of carbon dioxide and water vapor from N structures

$$- C + B$$

Vapor condensation and pool boiloff

SODIUM POOL MASS DIFFERENTIAL EQUATION

$$\frac{d}{dt} M_p = \text{sodium pool mass change in Cell J} \quad (3.0.2)$$

$= I_{Na}$	Input table for sodium spill
$+ L_{IJ} - L_{JK}$	Sodium recycle from Cell I or to Cell K
$- R_{Na + CO_2} - R_{Na + H_2O}$	Chemical reactions of sodium with carbon dioxide and water vapor
$+ R_C + R_{Na_2O}$	Chemical reaction products of carbon and sodium oxide (actually carried in the atmosphere mass balance)
$+ \sum_N R_{CO_2} + \sum_N R_{H_2O}$	Concrete releases of carbon dioxide and water vapor from N structures
$- R_{Na + Conc}$	Chemical reaction with concrete
$+ C - B$	Vapor condensation and pool boiloff

WATER POOL MASS DIFFERENTIAL EQUATION

$$\frac{d}{dt} M_w = \text{water pool mass change in Cell J} \quad (3.0.3)$$

$= I_{H_2O}$	Input mass for water pool
$+ C - B$	Vapor condensation and pool boiloff

ATMOSPHERE ENERGY DIFFERENTIAL EQUATION

$$\frac{d}{dt} U_a = \text{atmosphere energy change in Cell J} \quad (3.0.4)$$

$$= H_{Na} I_{Na} + H_{N_2 + O_2} I_{N_2 + O_2}$$

Input tables for sodium spray and gas injection have enthalpy effects

$$+ \sum_I H_{IJ} L_{IJ} - \sum_K H_{JK} L_{JK}$$

Enthalpy leakage from Cell I or to Cell K

$$+ Q_{Na + CO_2} + Q_{Na + O_2} + Q_{Na + H_2O}$$

Chemical reaction heat of sodium with carbon dioxide, oxygen and water vapor

$$+ Q_{Na_2O + H_2O}$$

Chemical reaction heat of sodium oxide with water vapor

$$+ Q_{H_2 + O_2}$$

Chemical reaction heat of hydrogen and oxygen

$$+ \sum_N U_{CO_2} R_{CO_2} + \sum_N U_{H_2O} R_{H_2O}$$

Concrete releases of carbon dioxide and water vapor from N structures have energy effects

$$- U_f C + U_g B$$

Vapor condensation and pool boiloff have energy effects

$$+ Q_{FP}$$

Fission product decay power

$$+ \sum_N Q_{HS}$$

Heat transfer from N structures

$$- Q_{SC}$$

Space cooler

POOL ENERGY DIFFERENTIAL EQUATION

$$\frac{d}{dt} U_p = (\text{sodium or water}) \text{ pool energy change in Cell J} \quad (3.0.5)$$

$$+ H_{Na} I_{Na} + U_{H_2O} I_{H_2O}$$

Input table for sodium spill has enthalpy effects; input mass for water pool implies energy effect

$$+ H_{IJ} L_{IJ} - H_{JK} L_{JK}$$

Sodium recycle from Cell I or to Cell K has enthalpy effect

$$+ Q_{Na + CO_2} + Q_{Na + H_2O}$$

Chemical reaction heat of sodium with carbon dioxide and water vapor

$$+ Q_{Na + H_2}$$

Chemical reaction heat of sodium with hydrogen

$$+ Q_{Na + Conc}$$

Chemical reaction heat of sodium with concrete

$$+ \sum_N U_{CO_2} R_{CO_2} + \sum_N U_{H_2O} R_{H_2O}$$

Concrete releases of carbon dioxide and water vapor from N structures into sodium pool have energy effects

$$+ U_f C - U_g B$$

Vapor condensation and pool boiloff have energy effects

$$+ Q_{FP}$$

Fission product decay power

$$+ \sum_N Q_{HS}$$

Heat transfer from N structures

3.1 DEBUG CASES 1 TO 4, SODIUM SPRAYS AND SPACE COOLER OPERATION

Debug Case 1 checks simultaneously the thermal effects of the following four independent situations:

1. In Cell A, spray hot sodium into the 100% nitrogen atmosphere.
2. In Cell B, spray hot sodium into the 97.8% nitrogen, 2.2% oxygen atmosphere.
3. In Cell C, cool the atmosphere by operating a space cooler.
4. In Cell D, nothing happens; but, the initial conditions of the cell can have either a dry or humid atmosphere.

Debug Case 2, 3 and 4 check these same situations, but in different cells. These four cases have no heat structures and no cell leakage and, therefore, are adiabatic. These cases check the operation of the following input data cards:

Cell data:	Cards 2, 4, 6 and 8
	Cards 3, 5, 7 and 9

Space-cooler data:	Cards 1700, 1800, 1900 and 2000
--------------------	---------------------------------

Each case uses all four cells provided in the code. Each cell has a different volume and initial condition in order to show the independence of the cells. Cases 1 to 4 rotate these four situations among the four cells.

3.1.1 Spray Hot Sodium into 100% Nitrogen

The situation with hot sodium sprayed into 100% nitrogen occurs in Cell A of Case 1. The code calculates the initial conditions of this cell first.

The initial conditions of Cell A are defined by input data on Card 2 in terms of its volume (1001 ft³), and the pressure (12.0 psia), temperature (123⁰F) and oxygen content (0.0% oxygen) of the atmosphere that fills this volume. Also, because Card 3 follows Card 2, the relative humidity of water vapor in this atmosphere is assumed to be zero (0.0% humidity). The code assumes that this atmosphere is saturated with sodium vapor because the oxygen content is zero and calculates the sodium saturation properties at 123⁰F: vapor pressure, $P_{Na} = 1 \times 10^{-11}$ psia; specific volume, $V_{Na} = 2.3 \times 10^{13}$ ft³/lb; and internal energy $U_{Na} = 2080.4$ Btu/lb. The mass of sodium vapor is then

p.B.2

p.A.5

$$\begin{aligned} M_{Na} &= V/V_{Na} \\ &= (1001 \text{ ft}^3)/(2.3 \times 10^{13} \text{ ft}^3/\text{lb}) = 4.3 \times 10^{-11} \text{ lb} \end{aligned} \quad (3.1.1)$$

Case 1,
p.2

The nitrogen partial pressure is the cell pressure less the sodium vapor pressure:

$$\begin{aligned} P_{N_2} &= P - P_{Na} \\ &= (12.0 \text{ psia}) - (1 \times 10^{-11} \text{ psia}) = 12.0 \text{ psia} \end{aligned} \quad (3.1.2)$$

The code uses the Ideal Gas Law with the Ideal Gas Constant of $R = 10.7314$ psia-ft³/lb-mole-⁰R to calculate the mass of nitrogen and oxygen. The mass of nitrogen is then

$$\begin{aligned} M_{N_2} &= \frac{P_{N_2} V W_{N_2}}{R T} \\ &= \frac{(12.0 \text{ psia})(1001 \text{ ft}^3)(28.016 \text{ lb/mole})}{(10.7314)(123 + 459.67^{\circ}\text{R})} = 53.82 \text{ lb} \end{aligned} \quad (3.1.3)$$

Case 1,
p.2

p.A.4

The code calculates the nitrogen energy at 123⁰F: $U_{N_2} = 21.15$ Btu/lb.

The initial energy of the cell atmosphere is the sum of the energies of the nitrogen and sodium vapor:

$$U = M_{N_2} U_{N_2} + M_{Na} U_{Na} \quad (3.1.4)$$

$$= (53.82 \text{ lb } N_2)(21.15 \text{ Btu/lb}) + (4.3 \times 10^{-11} \text{ lb } Na)(2080.4 \text{ Btu/lb})$$

$$= 1138.3 \text{ Btu}$$

p.B.2
Case 1,
p.2 Note that the code does not report this 1138.3 Btu energy of nitrogen and sodium. Instead, the code reports the sum of this energy of nitrogen and sodium (1138.3 Btu) and of the sodium spray (15,491.7 Btu) input on Card 3 as the initial energy of the atmosphere. Thus, the code reports 16,630.0 Btu.

p.B.2 The Cell A transient follows the accident conditions which are defined by input data on Card 3 in terms of the sodium spray mass (51.0 lb) and energy (15,491.7 Btu). This transient requires integration of the following portions of the mass and energy differential equations for the cell:

Atmosphere mass:

$$\frac{d}{dt} M_a = I_{Na} - C \quad (3.1.5)$$

Sodium pool mass:

$$\frac{d}{dt} M_p = C \quad (3.1.6)$$

Atmosphere energy:

$$\frac{d}{dt} U_a = H_{Na} I_{Na} - U_f C \quad (3.1.7)$$

Pool energy:

$$\frac{d}{dt} U_p = U_f C \quad (3.1.8)$$

This integration is done using the code assumptions that the atmosphere is at the same temperature as the pool and that the atmosphere is saturated with pool vapor. Equations (3.1.5) and (3.1.7) are integrated by iterating

on the new cell temperature until both equations are satisfied. For example, if an iteration has a too-high temperature (400°F), the cell atmosphere will have too much vapor (M_a has 53.82 lb N_2 and 8.4×10^{-6} lb Na), the pool will not have enough condensate (51.0 lb Na), and the calculated cell atmosphere will be too high ($U_a = 3796.5$ Btu, mainly N_2 energy). This iteration is done in the EMVBAL subroutine to satisfy the volume, mass and energy equations below.

Mass of sodium vapor from atmosphere volume:

$$M_{Na} = V/V_{Na} \quad (3.1.1)$$

Mass of sodium condensate by difference:

$$C = M_{Na,tot} - M_{Na} \quad (3.1.9)$$

Atmosphere energy by difference:

$$U_a = U_{a,tot} - U_f C \quad (3.1.10)$$

In the above equations, $M_{Na,tot}$ and $U_{a,tot}$ are temporary values for sodium mass and total energy of the atmosphere that result from adding the spray to the initial mass and energy. The iteration settled on 360.2°F as the new cell temperature, and this satisfies the integrated form of the differential equations as shown below.

Case 1,
p.3

Atmosphere mass:

$$M_a' = M_a + I_{Na} - C \quad (3.1.11)$$

$$= (53.82 \text{ lb } N_2 + 4 \times 10^{-11} \text{ lb Na}) + (51.0 \text{ lb Na}) - (51.0 \text{ lb Na})$$

$$= (\underline{53.82 \text{ lb } N_2} + \underline{2 \times 10^{-6} \text{ lb Na}})$$

Case 1,
p.3

Sodium pool mass:

$$M_p' = M_p + C \quad (3.1.12)$$

Case 1,
p.3

$$\begin{aligned} &= (0.0 \text{ lb Na}) + (51.0 \text{ lb Na}) \\ &= \underline{(51.0 \text{ lb Na})} \end{aligned}$$

Atmosphere energy:

$$U_a' = U_a + H_{Na} I_{Na} - U_f C \quad (3.1.13)$$

Case 1,
p.3

$$\begin{aligned} &= (1138.3 \text{ Btu}) + (15,491.7 \text{ Btu}) - (13,223.5 \text{ Btu}) \\ &= \underline{(3406.6 \text{ Btu})} \end{aligned}$$

Pool energy:

$$U_p' = U_p + U_f C \quad (3.1.14)$$

Case 1,
p.3

$$\begin{aligned} &= (0.0 \text{ Btu}) + 13,223.5 \text{ Btu} \\ &= \underline{(13,223.5 \text{ Btu})} \end{aligned}$$

The nitrogen pressure is calculated from the Ideal Gas Law by Equation (3.1.3) rearranged:

$$P_{N_2} = \frac{M_{N_2} R T}{V W_{N_2}} \quad (3.1.3)$$

$$\begin{aligned} &= \frac{(53.82 \text{ lb } N_2)(10.7314)(360.2 + 459.67^\circ R)}{(1001^3 \text{ ft})(28.016 \text{ lb/mole})} \\ &= 16.90 \text{ psia} \end{aligned}$$

The cell pressure is the sum of the nitrogen pressure and sodium vapor pressure:

$$\begin{aligned} P &= P_{N_2} + P_{Na} & (3.1.2) \\ &= (16.90 \text{ psia}) + (9 \times 10^{-7} \text{ psia}) \\ &= \underline{(16.90 \text{ psia})} \end{aligned}$$

Case 1,
p.3

This containment transient in Cell A is over in the first time step of the code. Thereafter, the cell conditions remain stationary.

3.1.2 Spray Hot Sodium into 97.8% Nitrogen - 2.2% Oxygen

The situation with hot sodium sprayed into 97.8% nitrogen, 2.2% oxygen occurs in Cell B of Case 1. This situation differs from that of the previous case by including the chemical reaction between sodium and oxygen. Again, the code calculates the initial conditions of this cell first.

The initial conditions of Cell B are defined by input data on Card 4 in terms of its volume (2020 ft³), and the pressure (23.0 psia), temperature (234.0°F) and oxygen content (2.2% oxygen) of the atmosphere that fills this volume. Also, because Card 5 follows Card 4, the relative humidity of water vapor in this atmosphere is assumed to be zero (0.0% humidity). The code assumes that this atmosphere has no sodium vapor because of the presence of oxygen. The oxygen partial pressure is the cell pressure times the oxygen content:

p.B.2

$$\begin{aligned} P_{O_2} &= P F_{O_2} & (3.1.15) \\ &= (23.0 \text{ psia})(0.022 \text{ mole fraction}) \\ &= (0.506 \text{ psia}) \end{aligned}$$

The mass oxygen is calculated from the Ideal Gas Law:

$$\begin{aligned}
 M_{O_2} &= \frac{P_{O_2} V W_{O_2}}{R T} & (3.1.16) \\
 &= \frac{(0.506 \text{ psia})(2020 \text{ ft}^3)(32.0 \text{ lb/mole})}{(10.7314)(234.0 + 459.67^\circ R)} \\
 &= (4.39 \text{ lb } O_2)
 \end{aligned}$$

Case 1,
p.2

The nitrogen partial pressure is the cell pressure less the oxygen partial pressure:

$$\begin{aligned}
 P_{N_2} &= P - P_{O_2} & (3.1.17) \\
 &= (23.0 \text{ psia}) - (0.506 \text{ psia}) \\
 &= (22.494 \text{ psia})
 \end{aligned}$$

The mass of nitrogen is again calculated from the Ideal Gas Law, Equation 3.1.3. The initial energy of the cell atmosphere is the sum of the energies of the nitrogen and oxygen:

$$\begin{aligned}
 U &= M_{N_2} U_{N_2} + M_{O_2} U_{O_2} & (3.1.18) \\
 &= (171.0 \text{ lb } N_2)(40.66 \text{ Btu/lb}) + (4.39 \text{ lb } O_2)(37.26 \text{ Btu/lb}) \\
 &= (7116.0 \text{ Btu})
 \end{aligned}$$

Note again that the code does not report this 7116 Btu energy of nitrogen and oxygen. Instead, the code reports the sum of this energy of nitrogen and oxygen (7116 Btu) and of the sodium spray (231,714 Btu) input on Card 5 as the initial energy of the atmosphere. Thus, the code reports 238,830 Btu.

p.B.2

Case 1,
p.2

The Cell B transient follows the accident conditions which are defined by input data on Card 5 in terms of the sodium spray mass (543 lb Na) and energy (231,714.39 Btu). This transient requires integration of the

p.B.2

following portions of the mass and energy differential equations for the cell:

Atmosphere mass:

$$\frac{d}{dt} M_a = I_{Na} - R_{Na + O_2} + R_{Na_2O} - C \quad (3.1.19)$$

Sodium pool mass:

$$\frac{d}{dt} M_p = C \quad (3.1.6)$$

Atmosphere energy:

$$\frac{d}{dt} U_a = H_{Na} I_{Na} + Q_{Na + O_2} - U_f C \quad (3.1.20)$$

Pool energy:

$$\frac{d}{dt} U_p = U_f C \quad (3.1.8)$$

The new feature of this case is the chemical reaction between sodium and oxygen, which introduces the mass terms of $R_{Na + O_2}$ and R_{Na_2O} of Equation (3.1.19) and the energy term of $Q_{Na + O_2}$ of Equation (3.1.20). This chemical reaction is

with the attendant stoichiometric relation of

$$4 (22.991 \text{ lb Na/mole}) + (32.0 \text{ lb } O_2/\text{mole}) = 2 (61.982 \text{ lb } Na_2O/\text{mole})$$

or

$$(91.694 \text{ lb Na}) + (32 \text{ lb } O_2) = (123.964 \text{ lb } Na_2O)$$

This case had 543 lb of sodium react with the 4.39 lb oxygen; obviously, there was an excess of sodium. The combining weights, based on the stoichiometric relation, are $R_{Na} = 12.62 \text{ lb sodium}$, $R_{O_2} = 4.39 \text{ lb}$

Case 1, oxygen, and $R_{Na_2O} = 17.02 \text{ lb}$ sodium oxide. The energy term, $Q_{Na + O_2}$ is calculated by using the heat of this chemical reaction, 5700 Btu/lb Na consumed.

$$\begin{aligned} Q_{Na + O_2} &= (12.62 \text{ lb Na})(5700 \text{ Btu/lb Na}) \\ &= (71,970 \text{ Btu}) \end{aligned}$$

The temporary values for sodium mass and total energy of the atmosphere that result from adding the spray and chemical reaction to the initial mass and energy are as follows:

$$\begin{aligned} M_{Na,tot} &= I_{Na} - R_{Na} & (3.1.22) \\ &= (543 \text{ lb Na}) - (12.62 \text{ lb Na}) \\ &= (\underline{530.4 \text{ lb Na}}) \end{aligned}$$

$$\begin{aligned} U_{a,tot} &= U_a + H_{Na} I_{Na} + Q_{Na + O_2} & (3.1.23) \\ &= (7116 \text{ Btu}) + (231,714 \text{ Btu}) + (71,970 \text{ Btu}) \\ &= (\underline{310,800 \text{ Btu}}) \end{aligned}$$

Again the EMBVAL subroutine iterates to satisfy the volume, mass and energy relations of Equations (3.1.1), (3.1.9) and (3.1.10). The atmosphere energy includes that of nitrogen, sodium and sodium oxide. The iteration settles on 1142.6°F as the new cell temperature. This temperature satisfies the integrated form of the differential equations as shown below.

Atmosphere mass:

$$M_a' = M_a + I_{Na} - R_{Na + O_2} + R_{Na_2O} - C \quad (3.1.24)$$

$$\begin{aligned} &= (171.0 \text{ lb } N_2 + 4.39 \text{ lb } O_2) + (543 \text{ lb } Na) \\ &- (12.62 \text{ lb } Na + 4.39 \text{ lb } O)_2 + (17.02 \text{ lb } Na_2O) - (528.6 \text{ lb } Na) \\ &= \underline{171.0 \text{ lb } N_2} + \underline{1.76 \text{ lb } Na} + 17.02 \text{ lb } Na_2O \end{aligned}$$

Case 1,
p.3

Sodium pool mass:

$$M_p' = M_p + C \quad (3.1.12)$$

$$\begin{aligned} &= (0.0 \text{ lb } Na) + (528.6 \text{ lb } Na) \\ &= \underline{(528.6 \text{ lb } Na)} \end{aligned}$$

Case 1,
p.3

Atmosphere energy:

$$U_a' = U_a + H_{Na} I_{Na} + Q_{Na + O_2} - U_f C \quad (3.1.25)$$

$$\begin{aligned} &= (7116 \text{ Btu}) + (231,714 \text{ Btu}) + (71,970 \text{ Btu}) \\ &- (264,120 \text{ Btu}) \\ &= \underline{(46,680 \text{ Btu})} \end{aligned}$$

Case 1,
p.3

Pool energy:

$$U_p' = U_p + U_f C \quad (3.1.14)$$

$$\begin{aligned} &= (0.0 \text{ Btu}) + (264,120 \text{ Btu}) \\ &= \underline{(264,120 \text{ Btu})} \end{aligned}$$

Case 1,
p.3

In this case the sodium pool occupies 10.5 ft^3 of the 2020 ft^3 cell so that the atmosphere volume is only 2009.5 ft^3 . This atmosphere volume is used in the Ideal Gas Law, Equation (3.1.3), to calculate the nitrogen pressure, $P_{N_2} = 52.25 \text{ psia}$. Again, the cell pressure is the sum of the nitrogen pressure and sodium vapor pressure, Equation (3.1.2).

$$P = P_{N_2} + P_{Na} \quad (3.1.2)$$

$$= (52.25 \text{ psia}) + (0.60 \text{ psia})$$

$$= (52.85 \text{ psia})$$

Case 1,
p.3

This containment transient in Cell B is over in the first time step of the code. Thereafter, the cell conditions remain stationary.

3.1.3 Operate a Space Cooler to Cool a Cell

p.B.2

The situation with the space cooler operating to cool the cell occurs in Cell C of Case 1. The initial conditions of Cell C are defined by input data on Card 6 in terms of its volume (4444 ft³), and the pressure (45.0 psia), temperature (456°F) and oxygen content (21% oxygen or the same as air) of the atmosphere that fills this volume. Again, because Card 7 follows Card 6, the relative humidity of water vapor in this atmosphere is assumed to be zero (0.0% humidity). With these initial conditions, the cell has 450.4 lb nitrogen and 136.8 lb oxygen, with a total energy of 46,587 Btu.

Case 1,
p.2

This case introduces the space cooler, which is assumed to operate according to the equation,

$$Q_{SC} = A + B (T_a - T_{sc}) \text{ for } t_1 \leq t \leq t_2 \quad (3.1.26)$$

so long as $T_a \geq T_{min}$ where Q_{SC} (Btu/hr) is the space-cooler duty at t (hr) time and T_a (°F) atmosphere temperature; A (Btu/hr) and B (Btu/hr-°F) are input parameters; T_{sc} (°F) is the input coolant temperature; t_1 and t_2 (hr) are the input start and stop times for the cooler, respectively; and T_{min} (°F) is the input minimum temperature for cooler operation. The input data on Card 1900 define these input data as follows:

$$Q_{SC} = \underline{4972.1} + \underline{85.804} (T_a - \underline{56.0}) \text{ for } \underline{0.1} \leq t \leq \underline{0.8} \text{ so long as } p.B.2$$

$$T_a \geq \underline{0.0}$$

This debug case was solved by modifying the differential equation for atmosphere energy to an equation for atmosphere temperature of the cell. The modification is apparent in the following equation:

$$\frac{dU_a}{dt} = M_a C_v \frac{dT_a}{dt} = -Q_{SC} = -A - B (T_a - T_{SC}) \quad (3.1.27)$$

The solution to this temperature differential equation gives the cell atmosphere temperature, T'_a , at the time t' as

$$T'_a = T_{SC} - \frac{A}{B} + \left[(T_{a_1} - T_{SC}) + \frac{A}{B} \right] \text{Exp} \left[\frac{-B}{M_a C_v} (t' - t_1) \right] \quad (3.1.28)$$

where, for this case, the total heat capacity at constant volume is

$$\begin{aligned} M_a C_v &= (450.4 \text{ lb } N_2)(0.1819 \text{ Btu/lb} - ^\circ\text{F}) + (136.8 \text{ lb } O_2)(0.1690 \text{ Btu/lb} - ^\circ\text{F}) \\ &= 105.06 \text{ Btu}/^\circ\text{F} \end{aligned}$$

and the initial temperature and time are $T_{a_1} = 456^\circ\text{F}$ and $t_1 = 0.10 \text{ hr}$, respectively.

At 0.60 hr, the cooler has been operating for 0.50 hr, and the cell temperature is $T'_a = \underline{302.5}^\circ\text{F}$. The cooler has removed the following energy: *Case 1,*
p.19

$$\begin{aligned} \int Q_{SC} dt &= M_a C_v (T_{a_1} - T'_a) \\ &= (105.06 \text{ Btu}/^\circ\text{F})(456 - 302.5^\circ\text{F}) \\ &= \underline{16,130 \text{ Btu}} \end{aligned} \quad (3.1.29)$$

Case 1,
p.19

If the cell atmosphere had contained water vapor, this cooler would have condensed and removed it. At 456°F, the cooler duty is, from Equation 3.1.26, $Q_{SC} = 39,294$ Btu/hr, and the internal energy for water vapor is

p.A.7

$U_{H_2O} = 1159$ Btu/lb. The water removal rate would have been

$$Q_{SC}/U_{H_2O} = 33.90 \text{ lb/hr}$$

and the atmosphere temperature would not have changed until all of the water vapor had been removed.

This space cooler operates up to 0.80 hours and cools the cell temperature to 255.6°F. Thereafter, the cooler stops and the cell temperature stays stationary.

Case 1,
p.25

3.1.4 Cell Independence

The situation with nothing happening occurs in Cell D of Case 1. The code calculates the initial conditions of this cell from the input data of Card 8 in terms of its volume (3456 ft³), and the pressure (34.0 psia), temperature (246°F) and oxygen content (3.3% oxygen) of the atmosphere that fills this volume. Also, because Card 9 follows Card 8, the relative humidity of water vapor in this Cell D atmosphere is assumed to be zero (0.0% humidity). With these initial conditions, the cell has 420.4 lb nitrogen and 16.4 lb oxygen.

p.B.2

Case 1,
p.2

The situation with nothing happening also occurs in Cell C of Case 2. Again the code calculates the initial conditions of this cell from input data of Card 6 which are identical to those listed above except, in this case, Card 7 precedes Card 6 and provides an input value for the relative humidity of water vapor in the cell atmosphere (44% relative humidity). The

p.B.3

code calculates the water saturation properties at 246°F : vapor pressure, $P_{\text{H}_2\text{O}} = 27.77 \text{ psia}$ and specific volume, $V_{\text{H}_2\text{O}} = 14.80 \text{ ft}^3/\text{lb}$. The mass of water vapor is then

p.A.7

$$M_{\text{H}_2\text{O}} = F_{\text{H}_2\text{O}} V/V_{\text{H}_2\text{O}} \quad (3.1.30)$$

$$= (0.44)(3426 \text{ ft}^3)/(14.80 \text{ ft}^3/\text{lb}) = \underline{102.7 \text{ lb}}$$

*Case 2,
p.3*

The water vapor partial pressure is the saturation value times the relative humidity:

$$P'_{\text{H}_2\text{O}} = F_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}} \quad (3.1.31)$$

$$= (0.44)(27.77 \text{ psia}) = \underline{12.22 \text{ psia}}$$

*Case 2,
p.3*

The partial pressure of nitrogen and oxygen is then

$$P_{\text{N}_2 + \text{O}_2} = P - P_{\text{H}_2\text{O}} \quad (3.1.32)$$

$$= (34.0 \text{ psia}) - (12.22 \text{ psia}) = 21.78 \text{ psia}$$

The code assumes that the oxygen partial pressure is based on this pressure of nitrogen and oxygen together (21.78 psia), not the cell pressure (34.0 psia). With this assumption, the oxygen partial pressure is

$$P_{\text{O}_2} = P_{\text{N}_2 + \text{O}_2} F_{\text{O}_2} \quad (3.1.33)$$

$$= (21.78 \text{ psia})(0.033 \text{ mole fraction})$$

$$= (0.719 \text{ psia})$$

The code continues with the calculation of oxygen mass (10.50 lb) and the nitrogen partial pressure (21.06 psia) and mass (269.30 lb). This code assumption modifies the oxygen content from the input data value (3.3%) to a smaller value (2.1%).

*Case 1,
p.3*

Debug Cases 2, 3 and 4 check the same situations as Case 1, but in different cells. These four situations and their summary results for Cases 1 through 4 are summarized in Table 3.1. These results show that in these situations the four cells are independent of one another.

p.B.2 These four debug cases are used to illustrate the effect that time step has on the results. The Card Series 9001 (Cards 9001, 9002, etc.) is used to input the appropriate values of time step for successive intervals of the analysis. The input value for the time step (0.0001 hr for Case 1) is used for the first 10 steps; then, the time step is increased in a succession of five steps, each by a factor of 1.58, to obtain the maximum step of 10 times the input step value. This succession of step increases makes the analysis run faster. With these adiabatic, no-leakage situations, the only one which is dependent upon the time step is that with the space cooler because the cooler is to have started at 0.10 hours and stopped at 0.80 hours. These start and stop times are not matched exactly; thus, there is some small variation in the final temperature of the cell illustrating this situation.

TABLE 3.1

DEBUG CASES 1 THROUGH 4

<u>Situation</u>	<u>Initial Sodium Spray</u>	<u>Initial Sodium Spray with Na-O₂ Reaction</u>	<u>Space Cooler Operation between 0.1 and 0.8 hr.</u>	<u>Initial Cell Conditions</u>	
Case 1	Cell A	Cell B	Cell C	Cell D	
Case 2	Cell D	Cell A	Cell B	Cell C	
Case 3	Cell C	Cell D	Cell A	Cell B	
Case 4	Cell B	Cell C	Cell D	Cell A	
Cell Volume, ft ³	<u>1001</u>	<u>2020</u>	<u>4444</u>	<u>3456</u>	<u>3456</u> p.B.2

	<u>Time 0.0 hr</u>	<u>Time 1 Step</u>	<u>Time 0.0 hr</u>	<u>Time 1 step</u>	<u>Time 0.1 hr</u>	<u>Time 0.8 hr</u>	<u>Time 0.0 hr</u>	<u>Time 0.0 hr</u>
Pressure, psia	<u>12.0</u>	<u>16.9</u>	<u>23.0</u>	<u>52.8</u>	<u>45.0</u>	<u>35.2</u>	<u>34.0</u>	<u>34.0</u>
Temperature, °F	<u>123.0</u>	<u>360.2</u>	<u>234.0</u>	<u>1142.6</u>	<u>456.0</u>	<u>255.6</u>	<u>246.0</u>	<u>246.0</u>
Nitrogen, lb	<u>53.8</u>	<u>53.8</u>	<u>17.1</u>	<u>17.1</u>	<u>450.4</u>	<u>450.4</u>	<u>269.3</u>	<u>420.4</u>
Oxygen, lb	<u>0.0</u>	<u>0.0</u>	<u>4.4</u>	<u>0.0</u>	<u>136.8</u>	<u>136.8</u>	<u>10.5</u>	<u>16.4</u>
Sodium, lb	<u>51.0</u>	<u>51.0</u>	<u>543.0</u>	<u>530.4</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>
Sodium oxide, lb	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>17.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>
Water, lb	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>102.7</u>	<u>0.0</u>
<i>Output for Cell A</i>	<i>Case 1</i>	<i>Case 1</i>	<i>Case 2</i>	<i>Case 2</i>	<i>Case 3</i>	<i>Case 3</i>	<i>Case 4</i>	<i>Case 1</i>
	<i>p. 2</i>	<i>p. 3</i>	<i>p. 3</i>	<i>p. 4</i>	<i>p. 2</i>	<i>p. 3</i>	<i>p. 3</i>	<i>p. 2</i>

3.2 DEBUG CASES 5 TO 8, SODIUM SPRAY AND SPILL AND AIR INJECTION

Debug Case 5 checks simultaneously the thermal effects of the following four independent situations:

- 1.) In Cell A, spray hot sodium into the 98.9% nitrogen, 1.1% oxygen atmosphere.
- 2.) In Cell D, spill hot sodium onto the floor under an atmosphere of 97.8% nitrogen, 2.2% oxygen.
- 3.) In Cell C, add air to pressurize and cool the 96.7% nitrogen, 3.3% oxygen atmosphere.
- 4.) In Cell B, nothing happens, but the initial conditions of the cell will activate either a sodium or water pool.

Debug Cases 6, 7 and 8 check these same situations, but in different cells. These four cases have no heat structures and no cell leakage and, therefore, are adiabatic. These cases check the operation of the following input data cards:

Cell data:	Cards 2, 4, 6 and 8 Cards 3, 5, 7 and 9
Sodium-spray data:	Card series 401, 501, 601 and 701
Sodium-spill data:	Card series 801, 901, 1001 and 1101
Air-injection data:	Card series 1201, 1301, 1401 and 1501

Each case uses all four cells provided in the code. Each cell has a different volume and initial conditions in order to continue to show the independence of the cells. Cases 5 to 8 rotate these four situations among the four cells.

3.2.1 Spray Hot Sodium Into 98.9% Nitrogen, 1.1% Oxygen

The situation with hot sodium sprayed into 98.9% nitrogen, 1.1% oxygen occurs in Cell A of Case 5. The initial conditions of this cell are defined by input data on Card 2 in terms of its volume (1234 ft³), and the pressure (12.0 psia), temperature (123⁰F) and oxygen content (1.1% oxygen) of the atmosphere that fills this volume. Also, because Card 3 follows Card 2, the relative humidity of water vapor in this atmosphere is assumed to be zero (0.0% humidity). Card 3 defines the surface area (8.5 ft²) of the sodium pool that may result from the sodium spray and the emissivity of the sodium pool surface (0.0) for radiation heat transfer from the pool surface to the atmosphere. These initial conditions provide 65.62 lb nitrogen and 0.834 lb oxygen, with an atmosphere energy of 1404 Btu.

p.B.6

p.B.6

Case 1,
p.3

The sodium spray into Cell A is defined by the Card Series 401 (Cards 401, 402, etc.). These cards input the data triplets of time (hr), sodium-spray rate (lb/hr) and sodium enthalpy (Btu/lb) and, thereby, describe any spray history desired. The spray history for the present case is shown in Figure 3.1: the spray begins at 0.10 hr with an enthalpy equivalent to liquid at 560⁰F, rises to a maximum rate of 16,667 lb/hr at 0.40 hr with an enthalpy equivalent to liquid at 500⁰F, and stops at 0.70 hr with an enthalpy equivalent to liquid at 440⁰F. An analytical representation of this spray history is derived for the CACECO check. This representation uses four time periods.

p.B.6

Period $0.0 \leq t \leq 0.1$ hr

Spray rate: $I_{Na} = 0.0$

Period $0.1 \leq t \leq 0.4$ hr

Spray rate: $I_{Na} = -5555.6 + 55,556.0 t$

Enthalpy: $H_{Na} = 328.83 - 62.667 t$

HEDL 7904-105.7

FIGURE 3.1. Sodium Spray History for Cell A of Debug Case 5.

Period $0.4 \leq t \leq 0.7$ hr

$$\text{Spray rate: } I_{\text{Na}} = 38,889.0 - 55,556.0 t$$

$$\text{Enthalpy: } H_{\text{Na}} = 329.04 - 63,200.0 t$$

Period $0.7 \leq t \leq 2.0$ hr

$$\text{Spray rate: } I_{\text{Na}} = 0.0$$

These representations are integrated to determine the quantity and energy of spray added to the cell. For example, if the spray rate were $I_{\text{Na}} = C + D t$, then the integral of this rate would be the quantity of spray added to the cell:

$$\int_{t_1}^{t_2} I_{\text{Na}} dt = C (t_2 - t_1) + \frac{D}{2} (t_2^2 - t_1^2)$$

Also, if the enthalpy were $H_{\text{Na}} = A + B t$, then the integral of the energy added to the cell would be

$$\int_{t_1}^{t_2} H_{\text{Na}} I_{\text{Na}} dt = AC (t_2 - t_1) + \frac{AD + BC}{2} (t_2^2 - t_1^2) + \frac{BD}{3} (t_2^3 - t_1^3)$$

The code assumes that the sodium spray mixed thoroughly with the atmosphere as it is added to the cell. This assumption causes the spray to react immediately with any carbon dioxide, hydrogen, oxygen and water vapor in the cell atmosphere. In particular, the reaction of the sodium spray with oxygen was discussed in Section 3.1.2 in connection with Equations (3.1.19) through (3.1.23).

From Equation (3.1.21), the first 2.40 lb of sodium spray will react all of the 0.834 lb oxygen in the cell and thereby add 744 Btu of spray

Case 5, energy, 13,655 Btu of chemical reaction energy, and 3.23 lb Na₂O to the
p.8 cell. This first part of the spray, which takes only the brief interval
from 0.100 to 0.109 hr, causes the maximum temperature in the cell. The
Case 5, chemical reaction heats the cell atmosphere to 1183°F and, thereafter,
p.10 further addition of the sodium spray only cools this atmosphere.

The spray was finished at 0.7 hr, with 5000 lb of sodium and 1,518,700 Btu of spray enthalpy added to the cell. The combined effect of sodium spray and chemical reaction was discussed in Section 3.1.2 for the situation wherein the spray lasted only one time step. In the present case, the spray lasts many time steps (for 0.6 hours), but the analysis is much the same. The temporary values for sodium mass and total energy of the atmosphere result from adding the spray and chemical reaction to the initial mass and energy. For example, the integrated results for the 0.6-hr spray are as follows:

$$M_{\text{Na,tot}} = I_{\text{Na}} - R_{\text{Na}} \quad (3.1.22)$$

$$= (5000 \text{ lb Na}) - (2.40 \text{ lb Na}) = (\underline{4997.60 \text{ lb Na}})$$

$$U_{\text{a,tot}} = U_{\text{a}} + H_{\text{Na}} I_{\text{Na}} + Q_{\text{Na}} + Q_2 \quad (3.1.23)$$

$$= (1404 \text{ Btu}) + (1,518,700 \text{ Btu}) + (13,655 \text{ Btu})$$

$$= (\underline{1,533,700 \text{ Btu}})$$

Case 5, Again, the EMBVAL subroutine iterates to satisfy the volume, mass and energy
p.29 relations of Equations (3.1.1), (3.1.9) and (3.1.10). The atmosphere energy
Case 5, includes that of nitrogen, sodium and sodium oxide. The iteration settles
p.29 on 505.9°F as the new cell temperature. This temperature satisfies the
integrated form of the differential equations as shown below.

$$M_a' = M_a + I_{Na} - R_{Na} + O_2 + R_{Na_2O} - C \quad (3.1.24)$$

$$\begin{aligned} &= (65.6 \text{ lb } N_2 + 0.83 \text{ lb } O_2) + (5000 \text{ lb } Na) \\ &- (2.40 \text{ lb } Na + 0.83 \text{ lb } O_2) + (3.23 \text{ lb } Na_2O) - (4997.60 \text{ lb } Na) \\ &= (\underline{65.6 \text{ lb } N_2} + \underline{1.5 \times 10^{-4} \text{ lb } Na}) \end{aligned} \quad \text{Case 5, p.29}$$

Sodium pool mass:

$$M_p' = M_p + C \quad (3.1.12)$$

$$\begin{aligned} &= (0.0 \text{ lb } Na) + (4997.60 \text{ lb } Na) \\ &= (\underline{4997.6 \text{ lb } Na}) \end{aligned} \quad \text{Case 5, p.29}$$

Atmosphere energy:

$$U_a' = U_a + H_{Na} I_{Na} + Q_{Na} + O_2 - U_f C \quad (3.1.25)$$

$$\begin{aligned} &= (1404 \text{ Btu}) + 1,518,700 \text{ Btu} + (13,655 \text{ Btu}) \\ &- (1,527,300 \text{ Btu}) \\ &= (\underline{6395 \text{ Btu}}) \end{aligned} \quad \text{Case 5, p.29}$$

Pool Energy:

$$U_p' = U_p + U_f C \quad (3.1.14)$$

$$\begin{aligned} &= (0.0 \text{ Btu}) + 1,527,300 \text{ Btu} \\ &= (\underline{1,527,300 \text{ Btu}}) \end{aligned} \quad \text{Case 5, p.29}$$

This containment transient in Cell A is over at 0.7 hours. Thereafter, the cell conditions remain stationary.

3.2.2 Spill Hot Sodium Into Cell With 97.8% Nitrogen - 2.2% Oxygen

The situation with hot sodium spilled into a cell with an atmosphere of 97.8% nitrogen and 2.2% oxygen occurs in Cell B of Case 5. The initial

p.B.6

conditions of this cell are defined by input data on Card 4 in terms of its volume (1000 ft³), and the pressure (23 psia), temperature (234⁰F) and oxygen content (2.2% oxygen) of the atmosphere that fills this volume.

n.B.6

Also, because Card 5 precedes Card 4, the relative humidity of water vapor in this atmosphere is defined to be zero (0.0% humidity). Card 5 also defines the surface area (9.5 ft²) of the sodium pool that will result from the sodium spill and the emissivity of the sodium pool surface (0.0) for radiation heat transfer from the pool surface to the atmosphere. These

Case 5,
p.3

initial conditions provide 84.66 lb nitrogen and 2.18 lb oxygen, with an atmosphere energy of 3523 Btu.

p.B.6

The sodium spill into Cell B is defined by the Card Series 901 (Cards 901, 902, etc.). These cards input the data triplets of time (hr), sodium-spill rate (lb/hr) and sodium temperature (⁰F) and, thereby, describe any spill history desired. The spill history for the present case is shown in Figure 3.2: the spill begins at 0.2 hr with a temperature of 600⁰F, rises to a maximum rate of 45,000 lb/hr at 0.6 hr with a temperature of 900⁰F, and then stops. An analytical representation of this spill history is derived for the CACECO check. This representation uses three time periods.

Period $0.0 \leq t \leq 0.2$ hr

Spill rate: $I_{Na} = 0.0$

Period $0.2 \leq t \leq 0.6$ hr

Spill rate: $I_{Na} = -22,500 + 112,500 t$

Temperature: $T_{Na} = 450 + 750 t$

Period $0.6 \leq t \leq 1.0$ hr

Spill rate: $I_{Na} = 0.0$

FIGURE 3.2. Sodium Spill History for Cell B of Debug Case 5.

These representations are integrated to determine the quantity and temperature of spill added to the cell.

The code assumes that the sodium spill goes into the sodium pool. Also, the code assumes that the atmosphere is at the same temperature as the pool and that the atmosphere is saturated with pool vapor. The net effect is to react the spill with any carbon dioxide, hydrogen, oxygen and water vapor in the cell atmosphere -- very much the same as if the spill were a spray. In this particular case, the first 6.25 lb of sodium spill will react all of the 2.18 lb oxygen in the cell and, thereby, add 2095 Btu of spill energy, 35,630 lb of chemical reaction energy, and 8.42 lb Na_2O to the cell. This first part of the spill, which takes only the brief interval from 0.200 to 0.2105 hr, causes the maximum temperature in the cell. The chemical reaction heats the cell temperature to about 2070°F and, thereafter, further addition of the sodium spill only cools this cell.

Case 5,
p.17

Case 5,
p.11

The spill is finished at 0.6 hr, with 9000 lb of sodium added to the cell at an average temperature of 796.9°F. The code assumes that this spill comes from within the cell, as if a tank inside the cell drained into the cell, so that the spill does not pressurize the cell by occupying space. The code affects this assumption by adding the spill volume to the cell volume. In this case, the 9000-lb spill at 796.9°F has an average density of 53.08 lb/ft³ so that the spill volume is 169.6 ft³. The cell volume after the spill is finished is its original volume (1000 ft³) plus the spill volume (169.6 ft³), or 1169.6 ft³.

p.4.5

Case 5,
p.23

The sodium spill forms a pool with a surface area (9.5 ft²) defined by input data. With a spill volume of 169.6 ft³, the pool is about 17.8 ft deep and is represented in the CACECO code analysis as a planar heat structure with seven temperature nodes uniformly spaced through the depth. In this situation, the temperature nodes are at 2.97-ft spacings.

Case 5,
p.23

The spill is finished at 0.6 hr, with 9000 lb of sodium and 3,558,000 Btu of spill enthalpy added to the cell. The effect of the chemical

reactions was discussed in Section 3.2.1. The iteration settles on 809.4°F *Case 5,*
as the new cell temperature. This containment transient is over at 0.6 hours. *p.23*
Thereafter, the cell conditions remain stationary.

3.2.3 Inject Cold Air into 96.7% Nitrogen - 3.3% Oxygen

The situation with cold air injected into 96.7% nitrogen, 3.3% oxygen atmosphere occurs in Cell C of Case 5. The initial conditions of this cell are defined by input data on Card 6 in terms of its volume (3456 ft³), and *p.B.6*
the pressure (34 psia), temperature (345°F) and oxygen content (3.3% oxygen) of the atmosphere that fills this volume. Also, because Card 7 follows Card 6, the relative humidity of water vapor in this atmosphere is assumed to be zero (0.0% humidity). These initial conditions provide 368.65 lb nitrogen and 14.37 lb oxygen, with an atmosphere energy of 23,120 Btu. *Case 5, p.3*

The air injected into Cell C is defined by the Card Series 1401 (Cards 1401, 1402, etc.). These cards input the data quadruplets of time (hr), gas-injection rate (lb/hr), gas temperature (°F) and oxygen content (% oxygen) and, thereby, describe any injection history desired. The injection history for the present case is shown in Figure 3.3: the injection begins at 0.40 hr with an injection rate of 2057.1 lb/hr at 80°F and 21% oxygen and continues at this rate and these conditions until 0.70 hr. *p.B.6*
An analytical representation of this injection history is derived from the CACECO check. The representation uses three time periods:

Period $0.0 \leq t \leq 0.4$ hr

Injection rate: $I_{N_2 + O_2} = 0.0$

Period $0.4 \leq t \leq 0.7$ hr

Injection rate: $I_{N_2 + O_2} = 2057.1$ lb/hr

Temperature: 80°F

Oxygen content: 21.0% oxygen

FIGURE 3.3. Air Injection History for Cell C of Debug Case 5.

Period $0.7 \leq t \leq 2.0$ hr

$$\text{Injection rate: } I_{N_2 + O_2} = 0.0$$

This transient requires integration of the following portions of the mass and energy differential equations for the cell:

Atmosphere mass:

$$\frac{d}{dt} M_a = I_{N_2 + O_2} \quad (3.2.1)$$

Atmosphere energy:

$$\frac{d}{dt} U_a = H_{N_2 + O_2} I_{N_2 + O_2} \quad (3.2.2)$$

The integration over the 0.3-hr injection results in the following equations:

Atmosphere mass:

$$\begin{aligned} M_a' &= M_a + I_{N_2 + O_2} \\ &= (368.65 \text{ lb } N_2 + 14.37 \text{ lb } O_2) + (473.40 \text{ lb } N_2 + 143.73 \text{ lb } O_2) \\ &= (842.05 \text{ lb } N_2 + 158.10 \text{ lb } O_2) \end{aligned} \quad (3.2.3)$$

Atmosphere energy:

$$\begin{aligned} U_a' &= U_a + H_{N_2 + O_2} I_{N_2 + O_2} \\ &= (23,120 \text{ Btu}) + (31,220 \text{ Btu}) \\ &= (54,340 \text{ Btu}) \end{aligned} \quad (3.2.4)$$

The EMVBAL subroutine iterates to determine the atmosphere temperature and settles on 314.5°F as the new cell temperature after the injection. This injection increases the oxygen concentration from the initial 3.3% to 14.12% and cools the cell from the initial 345°F to 314.5°F.

Case 5,
p. 29

An alternative analytical representation of this injection covers the oxygen mass balance. This representation uses two differential equations:

Atmosphere mass:

$$\frac{d}{dt} Ma = W \quad (3.2.5)$$

Oxygen mass:

$$\frac{d}{dt} (M_a C) = M_a \frac{dC}{dt} + WC = WC_i \quad (3.2.6)$$

In the two equations above, C represents the oxygen concentration in the cell, C_i the oxygen concentration in the injected air, and W the air-injection rate ($I_{N_2 + O_2}$ of Equation 3.2.1). The analytical solution of these two equations is difficult, and so a numerical solution was found using Euler integration method with time steps of 0.001 hr. This solution gives the cell concentration and mass as summarized below.

	<u>Time</u> <u>(hr)</u>	<u>Total</u> <u>Mass</u> <u>(lb moles)</u>	<u>Oxygen</u> <u>Concentration</u> <u>(%)</u>
<i>Case 5, p. 19</i>	<u>0.40</u>	13.608	<u>3.30</u>
<i>Case 5, p. 19</i>	<u>0.45</u>	17.173	<u>6.99</u>
<i>Case 5, p. 21</i>	<u>0.50</u>	20.738	<u>9.41</u>
<i>Case 5, p. 22</i>	<u>0.55</u>	24.302	<u>11.12</u>
<i>Case 5, p. 25</i>	<u>0.60</u>	27.867	<u>12.38</u>
<i>Case 5, p. 26</i>	<u>0.65</u>	31.432	<u>13.36</u>
<i>Case 5, p. 27</i>	<u>0.70</u>	34.997	<u>14.14</u>

The injection is finished at 0.70 hr. Thereafter, the cell conditions remain stationary.

3.2.4 Cell Independence

The situation with nothing happening occurs in Cell D of Case 5. The code calculates the initial conditions of this cell from the input data of Card 8 in terms of its volume (4567 ft³), and the pressure (45.0 psia), temperature (246⁰F) and oxygen content (4.4% oxygen) of the atmosphere that fills this volume. Also, Card 9 precedes Card 8 and provides input values for the relative humidity of water vapor in the cell atmosphere (87.585% relative humidity), the total water inventory of the cell ($I_{H_2O} =$ 33,643 lb water) and the liquid water energy of this inventory (7,218,100 Btu). The code calculates the water saturation properties at 246⁰F: vapor pressure (27.77 psia), specific volumes for liquid (0.01699 ft³/lb) and vapor (14.80 ft³/lb), and specific energies for liquid (214.55 Btu/lb) and vapor (1086.09 Btu/lb). Also, the code calculates the specific energies for nitrogen (42.79 Btu/lb) and oxygen (39.21 Btu/lb). Then, following the calculations outlined in Section 3.1.4, the code calculates the partial pressures, masses and energies of the water vapor, oxygen and nitrogen of the cell atmosphere.

p.B.6

p.B.6

p.A.7

p.A.4

<u>Material</u>	<u>Partial Pressure</u> (psia)	<u>Mass</u> (lb)	<u>Energy</u> (Btu)
Nitrogen	19.77	<u>334.00</u>	14,290
Oxygen	0.91	<u>17.56</u>	690
Water vapor	<u>24.32</u>	<u>270.24</u>	<u>293,500</u>
Total	<u>45.00</u>		<u>308,480</u>

*Case 5,
p.3*

*Case 5,
p.3*

The mass of pool water is the total water content less the mass in the atmosphere:

$$M_W = I_{H_2O} - M_a \quad (3.2.7)$$

$$= (33,643.00 \text{ lb}) - (270.24 \text{ lb}) = \underline{33,372.76 \text{ lb}}$$

*Case 5,
p.3*

The energy of this water pool is the input value less the energy of the mass that went into the atmosphere:

$$\begin{aligned} U_p &= U_{H_2O} I_{H_2O} - U_{H_2O} M_a & (3.2.8) \\ &= (7,218,100 \text{ Btu}) - (214.55 \text{ Btu/lb})(270.24 \text{ lb}) \\ &= \underline{7,160,100 \text{ Btu}} \end{aligned}$$

Case 5,
p.3

The volume occupied by this water pool is its mass times its specific volume:

$$\begin{aligned} V_p &= M_w V_{H_2O} & (3.2.9) \\ &= (33,372.8 \text{ lb water})(0.01699 \text{ ft}^3/\text{lb}) \\ &= (567 \text{ ft}^3) \end{aligned}$$

In these initial conditions, the cell atmosphere fills the whole of the cell volume of 4567 ft³ at the input pressure of 45 psia; the cell pool is abeyant -- it exists solely as mass and energy items. Then, in the first time step, the water pool is activated to fill its part of the cell volume, 567 ft³, which leaves only 4000 ft³ for the atmosphere. This activation of the water pool compresses the atmosphere to

$$\begin{aligned} P' &= P V/V' & (3.2.10) \\ &= (45.00 \text{ psia})(4567 \text{ ft}^3)/(4000 \text{ ft}^3) \\ &= \underline{51.38 \text{ psia}} \end{aligned}$$

Case 5,
p.4

This first time step also saturates the atmosphere with water vapor at 246°F. This saturation may cause heating or cooling of the cell depending upon whether water vapor is condensed or liquid water is evaporated. However, for the purposes of this debug case, the step causes no energy changes because the input value for relative humidity is the following volume ratio:

$$F_{H_2O} = V' / V = (4000 \text{ ft}^3) / (4567 \text{ ft}^3) = 0.87585$$

Debug Case 7 checks the same situation as this Case 5, but in Cell B.

The situation with nothing happening occurs in Cell A of Case 6, but this situation is different because a sodium pool is activated. Again the code calculates the initial conditions of this cell from the input data of Card 2 in terms of its volume (4567 ft³), and the pressure (45.00 psia), temperature (246°F) and oxygen content (0%) of the atmosphere that fills this volume. Also, Card 3 precedes Card 2 and provides input values for the relative humidity of water vapor in the cell atmosphere (0%), the liquid sodium inventory of the cell ($I_{Na} = \underline{32,660 \text{ lb sodium}}$) and the liquid sodium energy (7,256,700 Btu). The code calculates the sodium saturation properties at 246°F, including the specific volume for liquid (0.01736 ft³/lb) and the specific energy for nitrogen. Then, following the calculations outlined in Section 3.1.1, the code calculates the partial pressures, masses, and energies of the sodium vapor and nitrogen of the cell atmosphere:

<u>Material</u>	<u>Partial Pressure</u> (psia)	<u>Mass</u> (lb)	<u>Energy</u> (Btu)
Nitrogen	45.00	<u>760.31</u>	32,530
Sodium vapor	<u>1×10^{-8}</u>	<u>1×10^{-7}</u>	<u>0</u>
Total	<u>45.00</u>		<u>32,530</u>

Case 6,
p.4

Case 6,
p.4

The mass of pool sodium is the input datum

$$M_p = I_{Na} = \underline{32,660 \text{ lb}}$$

Case 6,
p.4

and the pool energy is the input datum

$$U_p = H_{Na} I_{Na} = \underline{7,256,700 \text{ Btu.}}$$

Case 6,
p.4

The volume occupied by this sodium pool is its mass times its specific volume:

$$V_p = M_p V_{Na} \quad (3.2.11)$$

$$= (32,600 \text{ lb sodium})(0.01736 \text{ ft}^3/\text{lb})$$

$$= (567 \text{ ft}^3)$$

Again, in these initial conditions the cell atmosphere fills the whole of the cell volume of 4567 ft^3 at the input pressure of 45 psia; the cell pool is abeyant -- it exists solely as mass and energy items. Then, again in the first time step, the sodium pool is activated to fill its part of the cell volume, 567 ft^3 , which compresses the atmosphere into the remaining volume of 4000 ft^3 and raises its pressure to 51.38 psia. Debug Case 8 checks the same situation as this Case 6, but in Cell C.

Case 6,
p.5

Debug Cases 6, 7 and 8 check the same situations as Case 5, but in different cells. These four situations and their summary results for Cases 5 through 8 are summarized in Table 3.2. These results show that in these situations, the four cells are independent of one another.

These four debug cases were used to illustrate the effect that time step has on the results. The Card Series 9001 (Cards 9001, 9002, etc.) is used to input the appropriate values of time step for successive intervals of the analysis. The input value for the time step (0.0001 hr for Case 5) is used for the first 10 steps; then, the time step is increased in a succession of five steps, each by a factor of 1.58, to obtain the maximum step of 10 times the input step value. This succession of step increases makes the analysis run faster. With these adiabatic, no-leakage situations, the spray, spill and air-injection processes are all dependent upon the start and stop times. Because these start and stop times are not matched exactly from case to case, there is some small variation in the final temperature of the cell illustrating each situation.

p.B.6

TABLE 3.2
DEBUG CASES 5 THROUGH 8

<u>Situation</u>	<u>Sodium Spray between 0.1 and 0.7 hr.</u>	<u>Sodium Spill between 0.2 and 0.6 hr.</u>	<u>Air Injection between 0.4 and 0.7 hr.</u>	<u>Initial Cell Conditions</u>	
Case 5	Cell A	Cell B	Cell C	Cell D	
Case 6	Cell B	Cell C	Cell D	Cell A	
Case 7	Cell C	Cell D	Cell A	Cell B	
Case 8	Cell D	Cell A	Cell B	Cell C	
Cell Volume, ft ³	<u>1234</u>	<u>1000</u> <u>1169.3</u>	<u>3456</u>	<u>4567</u> <u>4567</u>	p.B.6

43

	<u>Time 0.1 hr</u>	<u>Time 0.7 hr</u>	<u>Time 0.2 hr</u>	<u>Time 0.6 hr</u>	<u>Time 0.4 hr</u>	<u>Time 0.7 hr</u>	<u>Time 0.0 hr</u>	<u>Time 0.0 hr</u>
Pressure, psia	<u>12.0</u>	<u>21.2</u>	<u>23.0</u>	<u>41.2</u>	<u>34.0</u>	<u>84.1</u>	<u>45.0</u>	<u>45.0</u>
Temperature, °F	<u>123.0</u>	<u>505.9</u>	<u>234.0</u>	<u>809.4</u>	<u>345.0</u>	<u>314.5</u>	<u>246.0</u>	<u>246.0</u>
Nitrogen, lb	<u>65.6</u>	<u>65.6</u>	<u>84.6</u>	<u>84.6</u>	<u>368.6</u>	<u>842.0</u>	<u>334.0</u>	<u>760.3</u>
Oxygen, lb	<u>0.8</u>	<u>0.0</u>	<u>2.2</u>	<u>0.0</u>	<u>14.4</u>	<u>158.1</u>	<u>17.6</u>	<u>0.0</u>
Sodium, lb	<u>0.0</u>	<u>4997.6</u>	<u>0.0</u>	<u>8993.8</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>32,660.0</u>
Sodium oxide, lb	<u>0.0</u>	<u>3.2</u>	<u>0.0</u>	<u>8.4</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>
Water, lb	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>0.0</u>	<u>33,643.0</u>	<u>0.0</u>

<i>Output for Cell A</i>	<i>Case 5</i>	<i>Case 5</i>	<i>Case 8</i>	<i>Case 8</i>	<i>Case 7</i>	<i>Case 7</i>	<i>Case 5</i>	<i>Case 6</i>
	<i>p. 4</i>	<i>p.29</i>	<i>p. 5</i>	<i>p. 9</i>	<i>p. 5</i>	<i>p. 9</i>	<i>p. 3</i>	<i>p. 4</i>

3.3 DEBUG CASE 9, HEAT CONDUCTION IN PLANAR, CYLINDRICAL AND SPHERICAL HEAT STRUCTURES

Debug Case 9 checks the steady-state and transient-heat-conduction analyses of the heat structures which can be used to model the heat absorption characteristics of the roofs, walls, floors, and equipment of the cells. Each heat structure is described in the code by the one-dimensional, multi-region, transient-heat-conduction equation in planar, cylindrical, or spherical geometry. The case was designed so that the CACECO code results could be verified by comparison with analytical solutions which have been graphed by Carslaw and Jaeger.⁽²⁾ These analytical solutions cover the heating and cooling of one-dimensional planar, cylindrical, and spherical structures, both by a changed surface temperature and by a changed volumetric heat generation. All together these solutions cover many of the physical situations which are modeled in the application of the code to LMFBR facilities.

This case also checks the operation of the many different input data cards which are used to describe the characteristics of the heat structures and their heat transfer. In particular, this case uses 18 heat structures to check these input cards. The input cards, their numbers, and the structures affected are summarized below.

<u>Input Data Description</u>	<u>Card Numbers</u>	<u>Structure Numbers</u>
Cell temperature/constant temperature	Card 2	1, 8 / 11
	Card 4	2, 3, 6, 8 / 13
	Card 6	5, 14 / 4, 9
	Card 8	7, 10 / 12, 17
Decay power history	Card series 101	5, 6, 9, 10, 13, 14, 17, 18
Outside air temperature	Card series 1601	15, 16

<u>Data Description</u>	<u>Card Numbers</u>	<u>Structure Numbers</u>
Heat structure title	--	All 18
General information	1YY000*	All 18
Node locations	1YY100	All 18
Material numbers	1YY200	All 18
Volumetric heat distribution	1YY300	All 18
Boundary conditions	1YY400	All 18
Heat structure material data	Card series 300001	All 18
Constant heat-transfer coefficients	Card series 400001	1, 2, 9, 10, 18
Variable heat-transfer coefficients	Card series 410001 420001 430001 440001 450001 460001 470001 480001 490001	3, 13 8 7, 11 12, 15 6 4, 14 10 5 9
Heat structure initial temperature	YY*	1, 2, 3, 4, 7, 8 11, 12, 15, 16

* Note that the CACECO Users' Guide⁽¹⁾ uses YY to denote 01 for the first structure, 02 for the second structure, 03 for the third, etc.

The case was planned so that each analytical solution graphed by Carslaw and Jaeger could be checked by two sizes of heat structures: (1) a large size with a dimension of $l = \underline{2.19431 \text{ feet}}$ for the thickness of the slabs (planar structures) and for the radius of the cylinders and spheres and (2) a small size with a dimension of $l = \underline{0.69390 \text{ feet}}$ for the thickness

p.B.11

p.B.11

of the slabs and for the radius of the cylinders and spheres. Further, the case was planned so that all five materials used in the 18 structures had a thermal diffusivity of $\kappa = 0.4815 \text{ ft}^2/\text{hr}$, which was based on carbon steel. The Fourier Modulus combines the size of the structure, the thermal diffusivity of its material, and time, t in hours, in the dimensionless number $\kappa t/l^2$. For the large size of structure, this Modulus has the value of

$$\kappa t/l^2 = (0.4815 \text{ ft}^2/\text{hr})(t, \text{ hr})/(2.19431 \text{ ft})^2 = 0.1 t \quad (3.3.1)$$

and for the small size of structure, the Modulus has a value of $\kappa t/l^2 = 1.0 t$. Thus, during the time period from 0.1 to 1.0 hours, the Fourier Modulus advances from 0.01 to 0.1 for the large size of structure and from 0.1 to 1.0 for the small size of structure -- note the overlap. The CACECO code results for the large size of structure at 1.0 hour when its Fourier Modulus was $\kappa t/l^2 = 0.1$ should be the same as the code results for the small size of structure at 0.1 hour when its Modulus was $\kappa t/l^2 = 0.1$ also.

The general parameters checked by these 18 heat structures include 9 analytical solutions, 2 kinds of transients, 3 geometries, 5 values of thermal conductivity and 7 levels of volumetric heat power. These parameters are displayed below.

TABLE 3.3
SIMULATION PARAMETERS CHECKED BY CASE 9

Struc. Number	Carslaw and Jaeger ⁽²⁾		Cause of Transient	General Characteristics		Material Thermal Conductivity Btu/hr-ft-°F	Volumetric Heat Generation Btu/hr-ft ³
	Fig.	Page		Geometry	Size		
1	10B	98	(surface temperature)	planar	thick	26	--
2					thin	26	--
3	10C	98	(surface temperature)	planar	thick	6.5	--
4					thin	104	--
5	10D	98	(volumetric heat)	planar	thick	52	2160
6					thin	13	5400
7	11	101	(surface temperature)	planar	thick	26	--
8					thin	26	--
9	20	131	(volumetric heat)	planar	thick	104	4320
10					thin	6.5	2700
11	24	200	(surface temperature)	cylinder	large	13	--
12					small	52	--
13	26	205	(volumetric heat)	cylinder	large	52	4320
14					small	13	10800
15	29	234	(surface temperature)	sphere	large	6.5	--
16					small	104	--
17	32	244	(volumetric heat)	sphere	large	26	3240
18					small	26	32400

The CACECO parameters checked by these 18 heat structures include 3 levels of node numbers, 4 levels of region numbers, 3 kinds of volumetric heat distribution, 5 levels of left-boundary coordinate for planar structures, 2 boundaries active in heat transfer, 9 indices to the temperatures of cell atmosphere, constant source/sink, and outside air, and all 11 indices to heat-transfer coefficients, 9 of which are functions of time. These parameters are displayed below.

TABLE 3.4
CODE PARAMETERS CHECKED BY CASE 9

	Struc. Number	Number of Nodes	Number of Regions	Volumetric Heat Distribution	Left Bound. Coord. Feet	Boundary Specifications		
						Active Side	Bulk Temperature Index	Heat-Trans. Coefficient Index
<i>p.B.11</i>	1	<u>21</u>	<u>4</u>	--	<u>4.0</u>	right	<u>101</u>	<u>5</u>
	2	<u>11</u>	<u>3</u>	--	<u>0.0</u>	left	<u>104</u>	<u>6</u>
	3	<u>11</u>	<u>2</u>	--	<u>3.0</u>	right	<u>104</u>	<u>101</u>
	4	<u>6</u>	<u>1</u>	--	<u>1.0</u>	left	<u>109</u>	<u>106</u>
	5	<u>11</u>	<u>1</u>	all the same	<u>2.0</u>	right	<u>107</u>	<u>9</u>
	6	<u>11</u>	<u>4</u>	each region	<u>2.0</u>	left	<u>104</u>	<u>3</u>
<i>p.B.12</i>	7	<u>11</u>	<u>4</u>	--	<u>1.0</u>	right	<u>110</u>	<u>108</u>
	8	<u>11</u>	<u>1</u>	--	<u>3.0</u>	left	<u>101</u>	<u>105</u>
	9	<u>21</u>	<u>2</u>	each node	<u>0.0</u>	right	<u>109</u>	<u>103</u>
	10	<u>11</u>	<u>3</u>	each region	<u>4.0</u>	left	<u>110</u>	<u>102</u>
	11	<u>11</u>	<u>1</u>	--	<u>0.0</u>	right	<u>103</u>	<u>109</u>
	12	<u>11</u>	<u>4</u>	--	<u>0.0</u>	right	<u>112</u>	<u>107</u>
<i>p.B.13</i>	13	<u>11</u>	<u>3</u>	all the same	<u>0.0</u>	right	<u>106</u>	<u>103</u>
	14	<u>11</u>	<u>2</u>	each region	<u>0.0</u>	right	<u>107</u>	<u>104</u>
	15	<u>11</u>	<u>2</u>	--	<u>0.0</u>	right	<u>100</u>	<u>101</u>
	16	<u>11</u>	<u>3</u>	--	<u>0.0</u>	right	<u>100</u>	<u>106</u>
	17	<u>21</u>	<u>4</u>	each node	<u>0.0</u>	right	<u>112</u>	<u>104</u>
	18	<u>6</u>	<u>1</u>	each region	<u>0.0</u>	right	<u>104</u>	<u>3</u>

p.B.13 The five materials had the same thermal diffusivity. The nominal material was carbon steel with thermal conductivity of 26 Btu/hr-ft-⁰F and a volumetric heat capacity of 54 Btu/ft³-⁰F. The other four materials had conductivity and capacity values different by factors of 1/4, 1/2, 2 and 4 from the nominal value.

The code capability for analyzing heat conduction with volumetric heat generation was checked in 8 of the heat structures. This volumetric

heating depends upon the decay-power history, $\lambda(t)$, which is input on Card Series 101 and which, for this Case 9, had the constant value of $\lambda(t) = 1079.96 \text{ Btu/hr.}$ The code adjusts this decay power to volumetric power, A_0 , by using the following: the power factor, P_f , input as Word 6 of Card 1YY000; the time function, P_t , controlled by the time input as Word 7 of Card 1YY000; and the space distribution factors, $Q(X)$, input as either Word 3 of Card 1YY300 or as Words 2, 3, etc. of the Card Series 1YY301. The time function has value of either $P_t = 0$ or $P_t = 1$ and acts as a time switch to turn the volumetric heating either off or on. The Users' Guide description of the power factor and space-distribution factors assumes that the volume integral of distribution factors, $Q(X)$, over the heated volume of the structure, is unity; then, the power factor, P_f , is the reciprocal of this heated volume.⁽¹⁾ The volumetric power of the structure is the product

p.B.11

$$A_0 = \lambda(t) P_t P_f Q(X) \quad (3.3.2)$$

The power factor, space-distribution factor, and volumetric power for each of the 8 cases are listed in Table 3.5.

The steady-state temperature rise, ΔT , due to uniform volumetric heating depends upon the following: the volumetric power, A_0 ; the dimension of the structure, l ; its thermal conductivity, K ; and a geometric factor, f , which has a value of $f = 2$ for planar geometry, $f = 4$ for cylindrical, and $f = 6$ for spherical. This steady-state temperature rise is proportional to the dimensionless temperature, N_T :

$$N_T = \frac{K f \Delta T}{A_0 l^2} \quad (3.3.3)$$

This case was planned so that the steady-state temperature rise due to volumetric heating is $T = 100^\circ\text{f}$ for each of the 8 structures involved. That is, the dimensionless temperature is $N_T = 1$ for each case as shown below.

TABLE 3.5
VOLUMETRIC HEATING PARAMETERS OF CASE 9

Struc. Number	Power Factor P_f of 1YY000 card	Dist. Factor $Q(X)$ of 1YY301 cards	Volumetric Power A_0 Btu/hr-ft ³	Struc. Size, $\frac{1}{\text{feet}}$	Thermal Conductivity K Btu/hr-ft-°F	Geometry Factor f	Dimensionless Temperature $K f (100^\circ\text{F})$ $A_0 l^2$
5	1.0	2.0	2160	2.19431	52.0	2 (planar)	1.0
6	4.0	1.25	5400	0.69390	13.0	2	1.0
9	8.0	0.5	4320	2.19431	104.0	2	1.0
10	10.0	0.25	2700	0.69390	6.5	2	1.0
13	0.8	5.0	4320	2.19431	52.0	4 (cyl.)	1.0
14	20.0	0.5	10,800	0.69390	13.0	4	1.0
17	4.0	0.75	3240	2.19431	26.0	6 (sphere)	1.0
18	0.75	40.0	32,400	0.69390	26.0	6	1.0

For Structures 5 and 6, the volumetric heating is used to establish the initial temperature distribution; and, the time function, P_t , turns the volumetric heating off during the first time step. For the other structures, the time function turns the volumetric heating on during the first time step.

For each of the 18 heat structures, the temperature transient is a change of 100°F; but, this change is different for successive structures to show the independence of the boundary-temperature indices. For example, Structure 1 cools from 200°F to 100°F by using temperature index of 101 as input on Card 101400; Structure 2 cools from 300°F to 200°F by using index of 104 as input on Card 102400, etc. Further, the heat-transfer coefficients are different for successive structures to show the independence of the boundary-coefficient indices. For example, Structure 2 has coefficient $H(T, t) = \underline{2001 \text{ Btu/hr-ft}^2\text{-}^\circ\text{F}}$ by using the coefficient index of 6 as input on Card 102400; Structure 3 has coefficient $H(T, t) = \underline{750.1 \text{ Btu/hr-ft}^2\text{-}^\circ\text{F}}$ by using the coefficient index of 101 as input on Card 103400, etc. The

p.B.10

p.B.13

overall plan of this case was to demonstrate the precision of the code input for heat structures.

This case was planned so that the temperature drop, from the structure surface to the bulk temperature, would be about the same at the overlap condition for each structure pair. This plan utilized the boundary conditions of the CACECO code which combine the following: the thermal conductivity of the structure, K ; the temperature gradient at the structure surface, dT/dn ; the heat-transfer coefficient, $H(T, t)$; and the temperature drop from the surface to the bulk temperature, $T_s - T_b$:⁽¹⁾

$$-K \, dT/dn = H(T, t)(T_s - T_b) \quad (3.3.4)$$

At the overlap condition of $\kappa t/l^2 = 0.1$ for each structure pair (at 0.1 hr for the small structure and 1.0 hr for the large structure), the gradient should be the same; and, the coefficients were established so that the K/H ratio would be the same for each structure pair. For example, with Structures 13 and 14

Struc. Number	Thermal Conductivity K <u>Btu/hr-ft-°F</u>	Heat-Trans. Coefficient H <u>Btu/hr-ft²-°F</u>	<u>K/H Ratio ft</u>	
13	52	<u>3978</u>	0.013	Case 9, p.58
14	13	<u>1000</u>	0.013	Case 9, p.28

With the dT/dn gradient and the K/H ratio the same, the temperature drop should be the same. This plan was checked by calculating the temperature gradients at the overlap condition of each structure pair. This check, shown in Table 3.6, had the notable result that the temperature gradient for the small structure was about 3.1 times the gradient for the large structure of each pair. Nonetheless, the overall result was confirmation of the accuracy of the CACECO indices for heat-transfer coefficients.

TABLE 3.6
HEAT-TRANSFER COEFFICIENT CHECK OF CASE 9

	Struc. Number	Time hour	Heat-Transfer Coeff. CACECO Index	Value, H Btu/hr-ft ² -°F	Surf.-to-Bulk Temperature Dif. $ T_s - T_b $ °F	Gradients $H \frac{ T_s - T_b }{K}$ °F/ft	Ratio of these Gradients
<i>Case 9, p. 56</i>	1	1.0	5	1999	0.56	43	
<i>Case 9, p. 27</i>	2	0.1	6	<u>2001</u>	1.71	132	3.0
	3	1.0	101	758	0.52	61	
	4	0.1	106	<u>12,000</u>	1.66	191	3.2
	5	1.0	9	6000	0.50	58	
	6	0.1	3	<u>1000</u>	2.46	189	3.3
	7	1.0	108	4045	0.51	79	
<i>Case 9, p. 57</i>	8	0.1	105	<u>4000</u>	1.65	254	3.2
	9	1.0	103	3978	0.82	31	
<i>Case 9, p. 28</i>	10	0.1	102	<u>250</u>	2.47	95	3.0
	11	1.0	109	1517	0.47	55	
	12	0.1	107	<u>6000</u>	1.56	180	3.3
	13	1.0	103	3978	0.71	54	
	14	0.1	104	<u>1000</u>	2.18	168	3.1
	15	1.0	101	758	0.31	36	
<i>Case 9, p. 58</i>	16	0.1	106	<u>12,000</u>	1.03	119	3.3
	17	1.0	104	1989	0.91	70	
<i>Case 9, p. 29</i>	18	0.1	3	<u>1000</u>	5.48	211	3.0

If the CACECO results for Case 9 are compared with the analytical temperatures graphed by Carslaw and Jaeger⁽²⁾ in Figures 4 through 12, excellent agreement is shown. The particular test to note is the overlap condition for each structure pair at the Fourier Number $\kappa t/l^2 = 0.1$, which occurs for the small structure at $t = 0.1$ hr and for the large structure at $t = 1.0$ hr.

HEDL 7904-105.8

FIGURE 3.4. Comparison of CACECO and analytical temperatures in the slab $0 < x < 1$ with adiabatic boundary at $x = 0$, linear initial temperature and zero temperature at $x = 1$. The numbers on the curves are the values of $\kappa t/12$. The CACECO temperatures are shown by the bullets for Structure 1 and by the circles for Structure 2. The circled bullets indicate an overlap. Analytical temperatures are from Figure 10B, page 98 of Carslaw and Jaeger.⁽²⁾

HEDL 7904-105.9

FIGURE 3.5. Comparison of CACECO and analytical temperatures in the slab $0 < x < 1$ with adiabatic boundary at $x = 0$, linear initial temperature and zero temperature at $x = 1$. The numbers on the curves are the values of $\kappa t/l^2$. The CACECO temperatures are shown by the bullets for Structure 3 and by the circles for Structure 4. The circled bullets indicate an overlap. Analytical temperatures are from Figure 10C, page 98 of Carslaw and Jaeger.⁽²⁾

HEDL 7904-105.13

FIGURE 3.6. Comparison of CACECO and analytical temperatures in the slab $0 < x < 1$ with adiabatic boundary at $x = 0$, parabolic initial temperature and zero temperature at $x = 1$. The numbers on the curves are the values of $\kappa t/l^2$. The CACECO temperatures are shown by the bullets for Structure 5 and by the circles for Structure 6. The circled bullets indicate an overlap. Analytical temperatures are from Figure 10D, page 98 of Carslaw and Jaeger.⁽²⁾

FIGURE 3.7. Comparison of CACECO and analytical temperatures in the slab $0 < x < 1$ with adiabatic boundary at $x = 0$, zero initial temperature and temperature V at $x = 1$. The numbers on the curves are the values of $\kappa t/l^2$. The CACECO temperatures are shown by the bullets for Structure 7 and by the circles for Structure 8. Analytical temperatures are from Figure 11, page 101 of Carslaw and Jaeger.⁽²⁾

HEDL 7904-105.12

FIGURE 3.8. Comparison of CACECO and analytical temperatures in the slab $0 < x < 1$ with adiabatic boundary at $x = 0$, zero initial temperature and zero temperature at $x = 1$, and constant heat production at the rate of A_0 per unit volume. The numbers on the curves are the values of $\kappa t/l^2$. The CACECO temperatures are shown by the bullets for Structure 9 and by the circles for Structure 10. The circled bullets indicate an overlap. Analytical temperatures are from Figure 20, page 131 of Carslaw and Jaeger.⁽²⁾

HEDL 7904-105.3

FIGURE 3.9. Comparison of CACECO and analytical temperatures in the cylinder of radius a with zero initial temperature and surface temperature V . The numbers on the curves are the values of $\kappa t/a^2$. The CACECO temperatures are shown by the bullets for Structure 11 and by the circles for Structure 12. Analytical temperatures are from Figure 24, page 200 of Carslaw and Jaeger.⁽²⁾

HEDL 7904-105.11

FIGURE 3.10. Comparison of CACECO and analytical temperatures in the cylinder of radius a with zero initial temperature, zero surface temperature, and a constant heat production at the rate of A_0 per unit volume. The numbers on the curves are the values of $\kappa t/a^2$. The CACECO temperatures are shown by the bullets for Structure 13 and by the circles for Structure 14. The circled bullets indicate an overlap. Analytical temperatures are from Figure 26, page 205 of Carslaw and Jaeger.⁽²⁾

FIGURE 3.11. Comparison of CACECO and analytical temperatures in the sphere of radius a with zero initial temperature and surface temperature V . The numbers on the curves are the values of $\kappa t/a^2$. The CACECO temperatures are shown by the bullets for Structure 15 and by the circles for Structure 16. Analytical temperatures are from Figure 29, page 234 of Carslaw and Jaeger.⁽²⁾

HEDL 7904-105.10

FIGURE 3.12. Comparison of CACECO and analytical temperatures in the sphere of radius a with zero initial temperature, zero surface temperature, and constant heat production at the rate of A_0 per unit volume. The numbers on the curves are the values of $\kappa t/a^2$. The CACECO temperatures are shown by the bullets for Structure 17 and by the circles for Structure 18. The circled bullets indicate an overlap. Analytical temperatures are from Figure 32, page 244 of Carslaw and Jaeger.⁽²⁾

The CACECO code sums the heat-transfer rates for each boundary-temperature index, and these can be checked as illustrated in Table 3.7. According to the sign convention, a positive heat-transfer rate means that energy flows out of the heat structure into the atmosphere, pool or sink designated by the boundary-temperature index.

The CACECO code calculates the heat energy transferred from each structure by the integration of the heat-transfer rates over time. The energy transferred can also be calculated by hand from the change in sensible energy of each structure. The sensible energy is proportional to the volume integral (or average) of the temperature profile at the time of interest. This hand calculation does not provide high precision because of the author's difficulty in reading values of temperature from the graphs. Nevertheless, the effort substantiates the accuracy of the CACECO results as shown by the energy comparison in Table 3.8.

TABLE 3.7
CHECK CASE 9 SUMS OF HEAT-TRANSFER RATES

Struc. Number	Index 100	Heat-Transfer Rates at 1 Hour, Btu/hr							
		Index 101	Index 103	Index 104	Index 106	Index 107	Index 109	Index 110	Index 112
1		<u>20,246</u>							
2				<u>6,844</u>					
3				<u>6,271</u>					
4							<u>32,614</u>		
5						<u>41,600</u>			
6				<u>3,547</u>					
7								<u>-24,735</u>	
8		<u>-7,339</u>							
9							<u>32,481</u>		
10								<u>15,848</u>	
11			<u>-79,222</u>						
12									<u>-1,704</u>
13					<u>234,979</u>				
14						<u>81,672</u>			
15	<u>-56,147</u>								
16	<u>-40</u>								
17									<u>219,020</u>
18				<u>45,287</u>					
Sums	<u>-56,188</u>	<u>12,907</u>	<u>-79,222</u>	<u>61,751</u>	<u>234,979</u>	<u>123,273</u>	<u>65,096</u>	<u>-8,886</u>	<u>217,317</u>

Case 9,
p. 56

Case 9,
p. 57

Case 9,
p. 58

Case 9,
p. 58

TABLE 3.8

CHECK CASE 9 ENERGY TRANSFERS

		Analytical Solution, Carslaw and Jaeger				CACECO Results Energy Trans. at 1 hour	Apparent Difference %	
	Struc. Number	Figure No.	Curve $\kappa t/l^2$	Volume Integral of Temp.	Energy Scaled to CACECO Struc.			
Case 9, p. 56	1	10B	0.1	0.500-0.396	22,200 Btu	<u>21,592</u> Btu	2.7	
	2		1.0	0.500-0.043	29,100	<u>28,286</u>	2.8	
	3	10C	0.1	0.750-0.524	10,710	<u>10,305</u>	3.8	
	4		1.0	0.750-0.057	155,700	<u>149,496</u>	4.0	
	5	10D	0.1	0.662-0.512	49,800	<u>49,746</u>	0.1	
	6		1.0	0.662-0.057	14,700	<u>15,355</u>	4.3	
Case 9, p. 57	7	11	0.1	0.359	51,000	<u>47,868</u>	6.1	
	8		1.0	0.930	38,360	<u>36,236</u>	5.5	
	9	20	0.1	0.200-0.151	23,370	<u>20,282</u>	13.2	
	10		1.0	2.000-0.608	11,740	<u>11,514</u>	1.9	
	11	24	0.1	0.613	200,300	<u>188,651</u>	5.8	
	12		1.0	0.993	109,300	<u>107,839</u>	1.3	
	13	26	0.1	0.400-0.224	165,700	<u>160,844</u>	2.9	
	14		1.0	4.000-0.494	71,590	<u>70,513</u>	1.5	
	Case 9, p. 58	15	29	0.1	0.774	185,000	<u>176,623</u>	4.5
		16		1.0	1.000	90,690	<u>85,600</u>	5.6
17		32	0.1	0.600-0.253	165,800	<u>154,971</u>	6.5	
18			1.0	6.000-0.393	42,370	<u>41,780</u>	1.4	

The CACECO code also sums the energy transferred for each boundary-temperature index, and these can be checked by inspection as illustrated in Table 3.7 for the heat-transfer rates.

The heat structures can be used to model the roof, walls, floor and equipment of any cell and thereby simulate the heat exchange of these with the atmosphere and pool of each cell. The heat exchanges with the atmospheres of the four CACECO cells were checked in this case by modifying the differential equation for atmosphere energy to an equation for atmosphere temperature of the cell. The modification is apparent in the following equation:

$$\frac{dU_a}{dt} = M_a C_v \frac{dT_a}{dt} = \sum_N Q_{HS} \quad (3.3.5)$$

The solution to this temperature differential equation gives the cell atmosphere temperature, T'_a , at time t' :

$$T'_a = T_a + \frac{\int_t^{t'} \sum_N Q_{HS} dt}{M_a C_v} \quad (3.3.6)$$

The sums of the energy transferred are shown for each boundary-temperature index that denotes an atmosphere temperature. Again, according to the sign convention a positive energy transfer means that the energy transferred out of the heat structure into the atmosphere.

TABLE 3.9
CHECK CASE 9 SUMS OF ENERGY TRANSFERS

			Energy Transferred at 1 Hour, Btu			
Item			Cell A	Cell B	Cell C	Cell D
Boundary-temp. index			101	104	107	110
Case 9, p.56	Structure Number	1	<u>21,592</u>			
		2		<u>28,286</u>		
		3		<u>10,305</u>		
		5			<u>49,746</u>	
		6		<u>15,355</u>		
		7				<u>-47,868</u>
Case 9, p.57		8	<u>-36,236</u>			
		10				<u>11,514</u>
		14			<u>70,513</u>	
Case 9, p.58		18		<u>41,780</u>		
			_____	_____	_____	_____
Case 9, p.58	Sums:	$\int_t^{t'} \sum_N Q_{HS} dt$	<u>-14,645</u>	<u>95,726</u>	<u>120,258</u>	<u>-36,354</u>

The initial conditions of the four cells were different so that the cells held different amounts of nitrogen and oxygen at different temperatures. These atmosphere conditions are listed in Table 3.10.

TABLE 3.10
CASE 9 CELL ATMOSPHERES

<u>Item</u>	<u>Cell A</u>	<u>Cell B</u>	<u>Cell C</u>	<u>Cell D</u>	
Input Card	2	4	6	8	
Cell Volume, ft ³	<u>1,280,000</u>	<u>5,800,000</u>	<u>5,650,000</u>	<u>1,180,000</u>	<i>p.B.10</i>
Initial pressure, psia	<u>12.3</u>	<u>23.4</u>	<u>34.5</u>	<u>45.6</u>	
Initial temperature, °F	<u>100.00</u>	<u>200.00</u>	<u>300.00</u>	<u>400.00</u>	
Initial oxygen content, %	<u>1.2</u>	<u>1.4</u>	<u>1.6</u>	<u>1.8</u>	
Atmosphere mass, M _a , lbs	<u>73,565</u>	<u>538,184</u>	<u>671,397</u>	<u>163,824</u>	Case <i>Case 9,</i> <i>p.15</i>
Heat capacity, C _v , Btu/lb-°F	0.173	0.177	0.179	0.182	

The solutions for Equation 3.3.6 are shown below:

Cell A. $T'_a = (100.00^\circ\text{F}) + (-14,645 \text{ Btu}) / (73,565 \text{ lb})(0.173 \text{ Btu/lb-}^\circ\text{F})$ *Case 9,*
p.58
 $= (100.00) - (1.15) = \underline{(98.85^\circ\text{F})}$

Cell B. $T'_a = (200.00) + (+95,726) / (538,184)(0.177)$ *Case 9,*
p.58
 $= (200.00) + (1.00) = \underline{(201.00^\circ\text{F})}$

Cell C. $T'_a = (300.00) + (+120,258) / (671,397)(0.179)$ *Case 9,*
p.58
 $= (300.00) + (1.00) = \underline{(301.00^\circ\text{F})}$

Cell D. $T'_a = (400.00) + (-36,354) / (163,824)(0.182)$ *Case 9,*
p.59
 $= (400.00) - (1.22) = \underline{(398.78^\circ\text{F})}$

This Case 9 shows that CACECO provides accurate analyses of the heat structures, their energy transfers, and the energy effects in the cells. Overall, the check confirms the independence of the heat structures and of the cell atmospheres.

3.4 DEBUG CASE 10, HEAT CONDUCTION IN SODIUM POOLS AND ANALYSES WITH RADIATION

Debug Case 10 continues the check of the steady-state and transient-heat-conduction analyses of the heat structures which can be used to model the roofs, walls, floors, and equipment of the cells. This case concentrates on heat structures which are in thermal contact with the sodium or water pool of each cell and checks the CACECO representation of the sodium pool itself as a heat structure. Also, this case introduces radiation heat transfer between structures. The case was designed so that the CACECO code results could be verified by comparison with solutions provided by (a) Carslaw and Jaeger⁽³⁾ for the temperatures of a wall that cools a well-mixed pool and by (b) Zerkle and Sunderland⁽⁴⁾ for the temperatures of a pool or wall cooled by thermal radiation heat transfer. These solutions cover important physical situations which may be modeled in the application of the code to LMFBR facilities.

This case also continues the check of the many different input data cards which are used to describe the characteristics of the heat structures and their heat transfer. The input cards, their numbers, and the 10 structures affected are summarized below. Note that Structures 8, 9 and 10 are the sodium pools in Cells A, B and C respectively.

<u>Input Data Description</u>	<u>Card Numbers</u>	<u>Structure Numbers</u>
Cell conditions and pool formation	Cards 2 and 3	1, 8
	Cards 4 and 5	2, 3, 9
	Cards 6 and 7	4, 5, 6, 10
	Cards 8 and 9	7
Heat structure title	--	1 thru 7
General information	1YY000*	1 thru 7
Node locations	1YY100	1 thru 7
Material numbers	1YY200	1 thru 7
Volumetric heat distribution	1YY300	1 thru 7
Boundary conditions:	convection	Card 1YY400
	radiation	Card series 1YY401

<u>Input Data Description</u> (continued)	<u>Card Numbers</u>	<u>Structure Numbers</u>
Heat structure material data	Card series 300001	1 thru 7
Total interchange area	Card series 400001	2, 3, 9
Variable heat-transfer coefficients	Card series 410001	1
	Card series 440001	6, 10
	Card series 460001	5, 10
	Card series 450001	4, 10
	Card series 490001	7
Heat structure initial temperatures	YY*	1 thru 7

* Note that the CACECO Users' Guide⁽¹⁾ uses YY to denote 01 for the first structure, 02 for the second structure, 03 for the third, etc.

The general parameters checked by these 10 heat structures include 2 analytical solutions, 4 kinds of transients, 1 geometry, and 3 types of materials. These parameters are displayed below.

TABLE 3.11
SIMULATION PARAMETERS CHECKED BY CASE 10

<u>Struc. Number</u>	<u>Reference</u>	<u>Cause of Transient</u>	<u>Characteristics</u>		<u>Material</u>
			<u>Geometry</u>	<u>Size</u>	
1	Carslaw and Jaeger	convection heatup	planar	thin	basalt concrete
2	Zerkle and Sunderland	radiation heatup	planar	thin	carbon steel
3	Zerkle and Sunderland	radiation cooldown	planar	thin	carbon steel
4		convection heatup	planar	thin	basalt concrete
5				thick	stagnant sodium
6				thick	carbon steel
7	Carslaw and Jaeger	convection heatup	planar	thin	basalt concrete
8	Carslaw and Jaeger	convection cooldown	planar	thin	well-mixed sodium
9	Zerkle and Sunderland	radiation cooldown	planar	thick	stagnant sodium
10		convection cooldown	planar	thick	stagnant sodium

The CACECO parameters checked by these 10 heat structures include 4 levels of node numbers, 2 boundaries active in heat transfer, 2 modes of heat transfer, 9 indices to the temperatures of cell pools, constant source/sink, and other structures, and 7 indices to total interchange radiation areas or heat transfer coefficients, 5 of which are functions of time. These parameters are displayed below.

TABLE 3.12
CODE PARAMETERS CHECKED BY CASE 10

Struc. Number	Number of Nodes	Mode of Transfer	Boundary Specifications		
			Active Side	Temperature Index	Heat-Trans. Coeff. (Total Inter. Area) Index
1	<u>11</u>	convection	left	<u>102</u>	<u>101</u>
2	<u>7</u>	radiation	left	<u>-9</u>	<u>1</u>
3	<u>13</u>	radiation	left	<u>106</u>	<u>2</u>
4	<u>7</u>	convection	left	<u>+10</u>	<u>105</u>
5	<u>19</u>	convection	left	<u>+10</u>	<u>106</u>
6	<u>13</u>	convection	left	<u>+10</u>	<u>104</u>
7	<u>11</u>	convection	left	<u>111</u>	<u>109</u>
8	<u>7</u>	convection	mixed pool	--	--
9	<u>7</u>	radiation	top	<u>-2</u>	<u>1</u>
10	<u>7</u>	convection	bottom	<u>-4</u>	<u>105</u>
				<u>-5</u>	<u>106</u>
				<u>-6</u>	<u>104</u>

p.B.16

*Case 10,
p.6*

The variety of heat-transfer situations used in this Debug Case 10 are portrayed in Figure 3.13: in Cell A the sodium pool was cooled by the concrete floor; in Cell B the sodium pool was cooled by the steel roof; in Cell C the sodium pool was cooled by the concrete floor, the stagnant sodium floor and by the steel floor; and, in Cell D the water pool was cooled by the concrete floor. Note that the CACECO representation of the sodium pool as a heat structure permits both the top surface and bottom surface to be in convection contact with several other heat structures. This representation was checked by the sodium pool in Cell C, represented by Structure 10, which was in convection contact with Structures 4, 5 and 6.

FIGURE 3.13. Heat Structures for Debug Case 10.

The same situation is posed for the sodium pool in Cell A and for the water pool in Cell D: a hot pool is cooled by a cold concrete floor. This situation has an analytical solution provided by Carslaw and Jaeger⁽³⁾ which depends upon three dimensionless groups: the Fourier Number, $\kappa t/l^2$, the Nusselt Number, lH/K , and the heat-capacity ratio, $lA\rho C/M c'$. Definitions and appropriate values for the variables that make up these groups are listed below.

A, ft ²	Surface area of planar solid (basalt concrete floor)	
ρC , 30 <u>Btu/ft³-°F</u>	Volumetric heat capacity for solid	p.B.16
c' , Btu/lb-°F	Heat capacity for well-stirred fluid, either sodium or water	
H, <u>94.87 Btu/hr-ft²-°F</u>	Heat-transfer coefficient between fluid and solid	p.B.17 p.B.16
K, <u>1.2 Btu/hr-ft-°F</u>	Thermal conductivity of solid	
l, ft	Thickness of solid	
M lb	Mass of fluid	
t, hr	Time	
κ , 0.040 ft ² /hr	Thermal diffusivity of solid ($\kappa = K/\rho C$)	

The thickness of the concrete floor in each cell was set by having the Fourier Number equal to 0.1 at $t = 1$ hr; thus, $l = 0.63246$ ft. The heat-transfer coefficient was set by having the Nusselt Number equal to 50; thus, $H = 94.87$ Btu/hr-ft²-°F. The heat-capacity ratio was set so that the pools would cool to the mid-temperature in 1 hour. For the sodium pool spilled at 800°F onto 100°F concrete, the mid-temperature was 450°F; for the water pool spilled at 280°F onto 80°F concrete, the mid-temperature was 180°F. A few trials with the Carslaw and Jaeger equations and with CACECO established 2.50 as the appropriate value for the heat-capacity ratio and, thereby, the value 7.5895 Btu/ft²-°F for the associated ratio

of pool heat capacity to floor area ($M c' / A$). In Cell A with the sodium pool cooling from 800°F , $c' = 0.3099 \text{ Btu/lb-}^{\circ}\text{F}$, the average value for liquid sodium. In Cell D with the water pool cooling from 280°F , hand calculations showed that $c' = 1.0847 \text{ Btu/lb-}^{\circ}\text{F}$ to take into account the vapor condensation during the cool down. Thus, the spill mass to area ratio, M/A , was 24.490 lb/ft^2 for the sodium pool and 6.9969 lb/ft^2 for the water pool. With these ratios, the actual spill masses were adjusted so that the energy transfer would be about 10,000 Btu in 1 hour. Lastly, the volumes of both cells were the same, 10.31 ft^3 .

p.B.15

The CACECO input for establishing a sodium or water pool as an initial condition of a cell was described previously in Section 3.2.4. In the present case, Card 3 was used to spill 93.809 lb of sodium at 800°F into Cell A to form a pool with a surface area of 0.3403 ft^2 . Cell A, itself, was defined by Cards 3 and 2 as having a nitrogen atmosphere without oxygen or water vapor. Likewise, Card 9 was used to spill 93.518 lb of water at 280°F into Cell D to form a pool. Cell D, itself, was defined by Cards 9 and 8 as having a nitrogen atmosphere with $1.0\% \text{ oxygen}$ and water vapor of $84.6\% \text{ relative humidity}$.

p.B.15

p.B.15

Further, the CACECO input defined Structure 1 as the concrete floor of Cell A, with an area of 3.8304 ft^2 in contact with the average temperature of the sodium pool. Also, the input defined Structure 7 as the concrete floor of Cell D, with an area of 13.366 ft^2 in contact with the average temperature of the water pool. This assignment of the boundary temperature as being the average pool temperature was important for the sodium pool because, alternatively, the top or bottom surface temperatures of this pool could have been assigned.

p.B.16

The CACECO results for Cells A and D are summarized in Table 3.13. The beginning was taken at the first time step, 0.002 hr , because, as noted previously in Section 3.2.4, this first step may cause heating or cooling of cells having a pool as an initial condition.

TABLE 3.13
CACECO CHECK OF HOT POOL COOLED BY COLD FLOOR

Item	Cell A with Sodium Pool Cooled by Heat Structure 1		Cell D with Water Pool Cooled by Heat Structure 7	
	<u>0.002 hr*</u>	<u>1.000 hr**</u>	<u>0.002 hr***</u>	<u>1.000 hr****</u>
Cell temperature, °F (atmosphere and pool)	<u>799.2</u>	<u>456.5</u>	<u>279.8</u>	<u>181.6</u>
Nitrogen, lb	<u>0.2827</u>	<u>0.2827</u>	<u>0.7207</u>	<u>0.7207</u>
Oxygen, lb	<u>0.0000</u>	--	<u>0.0083</u>	<u>0.0083</u>
Sodium vapor, lb	<u>0.0002</u>	<u>0.0000</u>	--	--
liquid, lb	<u>93.8088</u>	<u>93.8090</u>	--	--
Water vapor, lb	--	--	<u>1.0066</u>	<u>0.1800</u>
liquid, lb	--	--	<u>92.5114</u>	<u>93.3380</u>
Atmosphere energy, Btu	<u>42</u>	<u>23</u>	<u>1,140</u>	<u>215</u>
Pool energy, Btu	<u>37,164</u>	<u>27,206</u>	<u>23,015</u>	<u>13,964</u>
Total cell energy, Btu	<u>37,205.5</u>	<u>27,229.3</u>	<u>24,155.2</u>	<u>14,178.8</u>
Cell energy loss, Btu	--	9,976.2	--	9,976.4
Floor surface temperature, °F	<u>105.8</u>	<u>448.2</u>	<u>81.2</u>	<u>179.3</u>
Floor sum of heat transfer (energy absorp- tion from start), Btu	<u>-23.7</u>	<u>-10,000</u>	<u>-23.4</u>	<u>-10,000</u>
Floor energy gain, Btu	--	9,976.2	--	9,976.4
Analytical solution for energy effect, Equation 3.4.2, Btu	296	10,078	296	10,048
Analytical Energy exchange, Btu	--	9,782	--	9,752

* Case 10, pp. 10-11
 ** Case 10, pp. 43-44
 *** Case 10, pp. 11-12
 **** Case 10, pp. 44-45

The CACECO code calculates the heat energy transferred from each structure by the integration of the heat-transfer rates over time. The code also sums the energy transferred for each boundary-temperature index, and these can be checked by inspection for Index 102 (Cell A pool) and for Index 111 (Cell D pool). With the CACECO code analysis, the energy balance between the atmosphere, pool, and all associated heat structures is accurate. The energy check is shown in Table 3.13 for both cells. The check involves the differential equation for atmosphere energy as well as the equation for pool energy because the code assumes that the atmosphere and pool are at the same temperature and that the atmosphere is saturated with pool vapor. That is, when the pool cools, the atmosphere cools as well. These two differential equations are added together below.

$$\frac{dU_a}{dt} + \frac{dU_p}{dt} = \sum_N Q_{HS} \quad (3.4.1)$$

The integral values of this equation are listed in Table 3.13:

U_a at 0.002 and 1.000 hr,

U_p at these same times, and

$\int_0^{1.0} \sum_1 Q_{HS} dt$ at these same times also.

Case 10 Thus, U_a (0.002 hr) = 42 Btu for the atmosphere, U_p (1.000 hr) = 27,206 Btu
pp. 11&44 for the sodium pool, and $\int_0^{1.0} \sum_1 Q_{HS} dt = \underline{+10,000 \text{ Btu}}$. For Cell A with the
p. 43 sodium pool, the cell energy loss to the floor was 9976.2 Btu and the energy absorption by the floor was 9976.2 Btu, an equality proving the accurate balance. Likewise for the Cell D with the water pool.

The CACECO temperatures for the cooling of the sodium pool in Cell A and the water pool in Cell D are confirmed by comparison with the analytical solution provided by Carslaw and Jaeger⁽³⁾ in Figure 3.14. The analytical solution was evaluated by the author, and six terms were sufficient for

HEDL 7904-105.6

FIGURE 3.14. Comparison of CACECO and analytical temperatures for the well-stirred fluid of V_0 initial temperature in contact with the slab of l thickness and zero initial temperature. The CACECO temperatures are shown by the bullets for the sodium pool of Cell A and by the circles for the water pool of Cell D. Analytical temperatures are from equations on page 317 of Carslaw and Jaeger.⁽²⁾

convergence of the infinite series in the equation for fluid temperature. The CACECO temperatures for the concrete floors under the sodium pool, Structure 1, and under the water pool, Structure 7, are confirmed by comparison with the analytical solution provided by Carslaw and Jaeger in Figure 3.15. The CACECO temperatures from the 11 temperature nodes of these heat structures are shown graphed at 0.1 hr, 0.4 hr, and 1.0 hr (at $\kappa t/l^2 = 0.01, 0.04$ and 0.1 , respectively). The analytical solution was evaluated by the author, and three terms were sufficient for convergence of the infinite series in the equation for solid temperature at $\kappa t/l^2 = 0.1$, six terms at $\kappa t/l^2 = 0.04$, and nine terms at $\kappa t/l^2 = 0.01$. This analytical solution for solid temperatures was operated on in order to evaluate the energy flow: (1) it was differentiated with respect to location to obtain the surface heat flux which (2) was integrated with respect to time to obtain the energy effect. The final equation is

$$E = -2\rho CL^2 V_0 \sum \frac{1.0}{P_s} \left[1.0 - \text{Exp}(-\alpha_s^2 \tau) \right] \quad (3.4.2)$$

where L is the Nusselt Number (lH/K), τ is the Fourier Number ($\kappa t/l^2$), and α_s and P_s are as defined by Carslaw and Jaeger⁽³⁾. This equation was evaluated by the author using thirty terms of the infinite series to estimate the converged values for E at $\tau = 0.0002$ and $\tau = 0.1$, which are listed in Table 3.13 at 0.002 and 1.0 hours, respectively. This analytical solution for the energy exchange from the hot pools to the cold floors confirmed the CACECO results. Overall, there is excellent agreement between the CACECO results and the analytical solution for this pool-cooling situation.

A different pool-cooling situation was posed in Cell B, which had the hot pool cooled by radiation heat transfer to a cold roof-wall heat sink. This radiation-cooling situation poses a nonlinear boundary condition to the transient-heat-conduction analysis and makes the analytical solution most difficult. The technical importance of the situation led Zerkle and Sunderland to study the problem by using a thermal-electrical analog computer and approximate analytical solutions.⁽⁶⁾ They presented their results in dimensionless, graphical form for a wide range of variables, and these charts were used to check the CACECO results.

FIGURE 3.15. Comparison of CACECO and analytical temperatures in the slab $0 \leq x \leq 1$ with zero initial temperature, adiabatic boundary at $x = 1$, and thermal contact with well-stirred fluid of V_0 initial temperature at $x = 0$. The numbers on the curves are the values of $\kappa t/l^2$. The CACECO temperatures are shown by the bullets for Structure 1 in contact with the sodium pool and by the circles for Structure 7 in contact with the water pool. Analytical temperatures are from equations of Page 317 of Carslaw and Jaeger.⁽²⁾

The Cell B sodium pool in its guise as Structure 9 and the steel slab of Structure 3 were planned in order to check the CACECO code in similar radiation-cooling situations. The cooling depends upon the following: the Fourier Number, N_{FO} (written by Zerkle and Sunderland as $N_{FO} = \alpha \gamma / L^2$); the ratio of environment temperature to initial slab temperature, T_e/T_i ; and the radiation number for cooling, $N_{rc} = K/\sigma F_{se} T_i^3 L$. The thicknesses of the sodium pool and steel slab were set by having the Fourier Number equal to $N_{FO} = 1.0$ at $t = 1$ hr; thus, $L_9 = 1.5972$ ft for the sodium pool (using $2.551 \text{ ft}^2/\text{hr}$ as the average thermal diffusivity), and $L_3 = 0.6939$ ft for the steel slab (using $0.4815 \text{ ft}^2/\text{hr}$ as thermal diffusivity). The environment and initial slab temperatures were set by having their ratio equal to $T_e/T_i = 0.50$ and by having the initial sodium and steel temperatures different. The selected temperatures are listed below.

p.B.16

	<u>Temperature</u>	<u>Sodium Pool</u>		<u>Steel Slab</u>	
		<u>°F</u>	<u>°R</u>	<u>°F</u>	<u>°R</u>
p.B.17	Initial slab, T_i	1000.00	1459.67	<u>1165.51</u>	1625.18
p.B.15	Environment, T_e	270.16	729.84	<u>352.92</u>	812.59

Finally, the radiation number for cooling was taken as equal to $N_{rc} = 0.30$ in order to realize a large temperature drop across the pool and slab. Such a low value for the radiation number usually implies a low value for the thermal conductivity of the slab, but, in this instance with sodium and steel, it means a high value for the total interchange factor, F_{se} . This interchange factor was set equal to $F_{se} = 16.986$ by the sodium pool condi-

Case 10,
p.11

p.B.16

p.B.17

tions (of $1,000^\circ\text{F}$ initial temperature, 1.5972 ft thickness and $43.36 \text{ Btu/hr-ft-}^\circ\text{F}$ for average thermal conductivity). For the steel slab with thermal conductivity of $K = 26 \text{ Btu/hr-ft-}^\circ\text{F}$ and thickness $L = 0.6939 \text{ ft}$, the same radiation number ($N_{rc} = 0.30$) and interchange factor ($F_{se} = 16.986$) set its initial temperature to 1165.51°F, as noted above.

Finally, the volume of the sodium and of the steel were each taken to be 10 ft^3 , which set the surface area of the sodium pool at 6.2610 ft^2 and the area of the steel slab at 14.411 ft^2 .

p.B.15

p.B.16

The CACECO input for establishing the sodium pool in Cell B uses Card 5 to spill 513.9 lb (10 ft^3) of sodium at $1,000^\circ\text{F}$ into the cell and to define the surface area of the pool to be 6.2610 ft^2 . The code acknowledges this area definition and sets up another heat structure, Structure 9, with planar geometry, and 7 uniformly spaced temperature nodes and appropriate boundary conditions. Material properties and thickness are calculated later as needed. Cell B itself is defined by Cards 5 and 4 as having a nitrogen atmosphere without oxygen or water vapor. Also, Card 4 defines the sink temperature, Index 106, with the value of 352.92°F to act as the environment temperature of the steel slab. Further CACECO input defines Structure 3 as the steel slab with an area of 14.411 ft^2 in radiation contact with the 352.92°F sink and an initial temperature of 1625.18°F . The 270.16°F environment temperature for the sodium pool is established by inventing a massive steel slab which would heat only 1°F in the process of cooling the pool for 1 hr. This slab is defined as Structure 2 with an area of 4509 ft^2 , a thickness of 0.36 ft , and an initial temperature of 269.66°F . Because the radiation boundary conditions of Structure 2 (defined on Card 102401) specifies the boundary temperature Index-9, the code automatically defines a radiation boundary condition of Structure 9 (the Cell B pool) as the boundary temperature Index-2; that is, the left surface of Structure 2 is in radiation contact with the top surface of Structure 9 and vice versa.

p.B.15

p.B.15

p.B.16

p.B.17

p.B.16

p.B.17

The final CACECO input for this radiation-cooling situation defines the total interchange areas for the cooling of the sodium pool and steel slab. These areas are denoted by $A_i F_{i,j}$. They were input on Card Series 400001 with the following values:

$$\text{Sodium pool: } A_9 F_{9,2} = A_9 F_{se} = (6.2610 \text{ ft}^2)(16.986) = \underline{106.35 \text{ ft}^2}.$$

p.B.16

$$\text{Steel slab: } A_3 F_{3,106} = A_3 F_{se} = (14.411 \text{ ft}^2)(16.986) = \underline{244.78 \text{ ft}^2}.$$

p.B.16

The code uses these total interchange areas to calculate, from the following equation, an equivalent heat-transfer coefficient for the radiation heat transfer from T_i to T_j :

$$H_r = (0.1713 \times 10^{-8} \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{R}^4)(A_i F_{i,j})(T_i^2 + T_j^2)(T_i + T_j)/A_i \quad (3.4.3)$$

Case 10,
p.22
p.21 For example, with the sodium pool to steel sink at 0.1 hr, the pool surface temperature is 556.58⁰F ($T_g = 1,016.25^{\circ}\text{R}$), the steel slab surface is 270.08⁰F ($T_3 = 729.75^{\circ}\text{R}$), and the equivalent heat-transfer coefficients are as follows:

For Structure 9, the sodium pool at 0.1 hr,

$$H_{r9} = (0.1713 \times 10^{-8})(106.35)(1016.25^2 + 729.75^2)(1016.25 + 729.75)/6.2610$$

Case 10,
p.22 = 79.52 Btu/hr-ft²-⁰F

For Structure 2, the steel sink,

$$H_{r2} = (0.1713 \times 10^{-8})(106.35)(1016.25^2 + 729.75^2)(1016.25 + 729.75)/4509.0$$

Case 10,
p.21 = 0.1104 Btu/hr-ft²-⁰F.

The code calculates the heat-transfer rate for each boundary condition from the following equation:

$$Q_{HS} = H A (T_i - T_j) \quad (3.4.4)$$

In this example, for the sodium pool at 0.1 hr,

$$Q_{HS9} = (79.52 \text{ Btu/hr-ft}^2\text{-}^{\circ}\text{F})(6.2610_{\text{ft}}^2)(556.58 - 270.08)$$

Case 10,
p.22 = 142,646 Btu/hr, a heat loss rate from the pool.

For the steel sink,

$$Q_{HS2} = (0.1104)(4509.0)(270.08 - 556.58)$$

Case 10,
p.21 = -142,646 Btu/hr, a heat gain rate to the slab.

The CACECO results for Cell B and Structures 2, 3 and 9 are summarized in Table 3.14. Again, the beginning was taken at the first time step, 0.002 hr, because this first step could have caused heating or cooling of the cell with a pool as an initial condition. Note that the table lists two temperatures for the sodium pool in each time column. For example, at 0.002 hr the cell temperature is 996.4°F, and the Structure 9 average temperature is 990.9°F. These two temperatures are justified as follows:

*Case 10,
p.11*

TABLE 3.14
CACECO CHECK OF HOT POOL COOLED BY RADIATION

Item	Cell B with Sodium Pool as Heat Structure 9		Heat Structure 2		Heat Structure 3	
	<u>0.002 hr*</u>	<u>1.000 hr**</u>	<u>0.002 hr***</u>	<u>1.000 hr****</u>	<u>0.002 hr***</u>	<u>1.000 hr****</u>
Cell temperature, °F (atmosphere and pool)	<u>996.4</u>	<u>448.6</u>				
Atmosphere energy, Btu	<u>482</u>	<u>188</u>				
Pool energy, Btu	<u>234,206</u>	<u>147,762</u>				
Total cell energy, Btu	<u>234,688</u>	<u>147,950</u>				
Cell energy loss, Btu	--	86,738				
Heat Structure Temperatures						
Active surface, °F	<u>897.4</u>	<u>373.8</u>	<u>269.83</u>	<u>270.72</u>	<u>992.0</u>	<u>471.6</u>
Mid plane, °F	<u>1,000.0</u>	<u>455.5</u>	<u>269.66</u>	<u>270.67</u>	<u>1,165.5</u>	<u>572.7</u>
Adiabatic surface, °F	<u>1,000.0</u>	<u>485.8</u>	<u>269.66</u>	<u>270.66</u>	<u>1,165.5</u>	<u>610.5</u>
Average, °F	990.9	446.4	269.68	270.68	1,156.4	561.9
Structure sum of heat transfer (energy absorption from start), Btu	<u>+566</u>	<u>+87,304</u>	<u>-566</u>	<u>-87,304</u>	<u>+1,680</u>	<u>+321,530</u>
Structure energy change, Btu	--	+86,738	--	-86,738	--	+319,850

* Case 10, p. 11

** Case 10, p. 44

*** Case 10, p. 10

**** Case 10, p. 43

1. 996.4°F is the cell temperature. It is the atmosphere-pool temperature resulting from the pool energy balance and the processes of Subroutine EMVBAL. This single value is taken as the correct, average temperature of the well-mixed pool and is the pool temperature used by all code processes that do not specifically designate the top or bottom surface temperatures of the sodium pool. In particular, this is the pool temperature designated by the boundary temperature Indices of 102 (used in this Case 10 for the Cell A sodium pool), 105, 108 and 111 (used in this Case 10 for the Cell D water pool).
2. 990.9°F is the trapezoidal average of the 7 nodal temperatures of the sodium pool heat structure. At each time step, just prior to the solution of the transient heat conduction equations for all of the heat structures, this trapezoidal average is calculated in Subroutine HP00L and then the 7 nodal temperatures are corrected for their apparent bias. For example, with the cell B sodium pool at 0.002 hr, the apparent bias is

$$996.4^{\circ} - 990.9^{\circ}\text{F} = 5.5^{\circ}\text{F}$$

and the corrected nodal temperatures are as indicated in the following tabulation:

STRUCTURE 9 AT 0.002 hr

<u>Node</u>	<u>Designation</u>	<u>Value</u>	<u>Corrected Value</u>
1	active surface	<u>897.4°F</u>	902.9°F
4	mid plane	<u>1000.0</u>	1005.5
7	adiabatic surface	<u>1000.0</u>	1005.5

*Case 10,
p.11*

The code author resolved the dichotomy of two average sodium-pool temperatures by using the temperature provided by Subroutine EMVBAL as the fiducial

value and adjusting the associated heat-structure temperatures to match. This resolution, unfortunately, sometimes leads to unusual pool heat-structure temperatures as will be illustrated later with Cell C.

Table 14 lists the energy changes from 0.002 hr to 1.000 hr for (1) Cell B, (2) Structure 9 (sodium pool of Cell B), and (3) Structure 2 as the magnitude 86,738 Btu. This energy was radiated from Structure 9 to Structure 2. The code convention calls for the heat loss from a structure to be a positive value and a heat gain to be a negative value; that is, +86,738 Btu loss by Structure 9, -86,738 Btu gain by Structure 2. The code energy balances are accurate.

The energy balances of the atmosphere and pool of the cell and of the associated heat structures are of sufficient importance to justify further checks. For example, the pool energy loss can be calculated by using the pool temperatures or the average structure temperatures in the following equation for times t_1 to t_2 :

$$U_p(t_1) - U_p(t_2) = M c' (T_1 - T_2) \quad (3.4.5)$$

For the Cell B pool temperatures,

$$\begin{aligned} U_p(t_1) - U_p(t_2) &= (513.9 \text{ lb})(0.3071 \text{ Btu/lb-}^{\circ}\text{F})(996.4^{\circ} - 448.6^{\circ}\text{F}) \\ &= (86,453 \text{ Btu}), \text{ which is within 0.3\% of} \\ &\text{the CACECO value listed in Table 3.14.} \end{aligned}$$

For the Structure 9 nodal temperatures,

$$\begin{aligned} U_p(t_1) - U_p(t_2) &= (513.9)(0.3071)(990.9^{\circ}\text{F} - 446.4^{\circ}\text{F}) \\ &= (85,932 \text{ Btu}), \text{ which is within 0.9\% of the} \\ &\text{CACECO value listed in Table 3.14.} \end{aligned}$$

Similarly, the steel structure energy changes can be calculated by using their average temperatures in the following equation for times t_1 to t_2 :

$$U_s(t_1) - U_s(t_2) = 1A \rho c (T_1 - T_2) \quad (3.4.6)$$

For Structure 2, the 270° sink,

$$\begin{aligned} U_s(t_1) - U_s(t_2) &= (0.36 \text{ ft})(4509 \text{ ft}^2)(54.0 \text{ Btu/ft}^3 - ^\circ\text{F})(269.68^\circ\text{F} - 270.68^\circ\text{F}) \\ &= (-87,655 \text{ Btu}), \text{ which is within 1.0\% of} \\ &\quad \text{the CACECO value listed in Table 3.14.} \end{aligned}$$

For Structure 3, the 1165° slab cooled by radiation,

$$\begin{aligned} U_s(t_1) - U_s(t_2) &= (0.69390)(14.411)(54.0)(1156.4^\circ\text{F} - 561.9^\circ\text{F}) \\ &= (321,012 \text{ Btu}), \text{ which is within 0.4\% of} \\ &\quad \text{the CACECO value listed in Table 3.14.} \end{aligned}$$

These checks confirm that the code energy balances are correct.

These CACECO temperatures for the cooling of the Cell B sodium-pool heat Structure 9 and of the steel slab Structure 3 are confirmed by comparison with the temperatures published by Zerkle and Sunderland⁽⁴⁾ in Figure 3.16. The CACECO temperatures of Nodes 1, 4 and 7 of Structure 9 and of Nodes 1, 7 and 13 of Structure 3 are shown graphed on the respective charts of the cooled face, center-plane, and insulated face of the slab. The CACECO results cover the line at $N_{rc} = 0.3$ from $N_{Fo} = 0.1$ to 1.0 as planned. There is excellent agreement between the CACECO results and the published solution for this radiation-cooling situation.

Another pool-cooling situation was posed in Cell C which had the hot sodium pool cooled by convection heat transfer to three floors. This situation was planned to check the CACECO facility for the sodium pool heat structure which permits up to 4 other heat structures to be in convection contact with the pool top surface and up to 5 other heat structures to be in contact with the bottom surface. Only the sodium-pool heat structures have this facility; the other structures which model the roof, walls, floor and equipment of the cells can be in convection contact with only one boundary temperature at each surface.

Transient temperature at the insulated face of a slab subjected to radiant cooling when $T_e/T_i = 0.50$.

Transient temperature at the center-plane of a slab subjected to radiant cooling when $T_e/T_i = 0.50$.

Transient temperature at the cooled face of a slab subjected to radiant cooling when $T_e/T_i = 0.50$.

HEDL 7904-105.2

FIGURE 3.16. Comparison of CACECO and published temperatures for the slab of $\leq x \leq L$ with adiabatic boundary at $x = L$, initial temperature $T_e = 0.50 T_i$. The numbers on the curves are the radiation numbers for cooling, $K/\sigma F_{se} T_i^3 L$. The CACECO temperatures are shown by the bullets for Structure 3 (sodium pool of Cell B) and by the circles for Structure 4 (steel slab). The circled bullets indicate an overlap. The published temperatures were graphed by Zerkle and Sunderland⁽⁴⁾ from their analytical and analog computer calculations.

The Cell C sodium pool cooling was planned so that

- (1) the pool would cool from 500°F as the floors heated from 100°F;
- (2) the total heat capacity of the pool would equal the sum of the total heat capacities of the three floors; that is, the pool would cool to 300°F as the floors heated to 300°F;
- (3) the three floors would have equal total heat capacities, which would be 1/3rd that of the pool;
- (4) the heat transfer into each floor would be the same;
- (5) the floors would be of different materials; and,
- (6) the structure thicknesses would be such that the Fourier Numbers would all be equal to 0.1 at 1 hr.

This planning resulted in the parameter values listed in Table 3.15. With these data, the total heat capacity of the pool was 9124 Btu/°F, the total heat capacity of each floor structure was 3035.8 Btu/°F, and the product of area and heat-transfer coefficient for each floor was 8000 Btu/hr-°F.

The CACECO input for establishing the sodium pool in Cell C uses Card 7 to spill 28,548 lbs of sodium at 500°F into the cell and to define the surface area of the pool to be 100 ft². Again, the code acknowledges this area definition and sets up another heat structure, Structure 10, with planar geometry, and 7 uniformly spaced temperature nodes and appropriate boundary conditions. Material properties and thickness are calculated later as needed. Cell C is defined by Cards 7 and 6 as having a nitrogen atmosphere without oxygen or water vapor. Further CACECO input defines Structure 4 as the concrete floor, Structure 5 as the stagnant sodium floor, and Structure 6 as the steel floor, all with areas, thicknesses, material properties, and heat-transfer coefficients as listed in Table 3.15. Because the convection boundary conditions of Structure 4 (defined on Card 104400) specify the boundary temperature Index +10, the code automatically defines a convection boundary condition of Structure 10 (the Cell C pool) as the boundary temperature Index -4; that is, the left surface of Structure 4 was in convection contact with the bottom surface of Structure 10, and vice versa. Likewise for Structure 5 (Card 105400) and for Structure 6 (Card 106400).

p.B.15

TABLE 3.15

CELL C POOL COOLING PARAMETERS

<u>Material</u>	<u>Heat Structure</u>	<u>Thermal Conductivity Btu/hr-ft-°F</u>	<u>Volumetric Heat Capacity Btu/ft³-°F</u>	<u>Thermal Diffusivity ft²/hr</u>	<u>Thickness ft</u>	<u>Area ft²</u>	<u>Heat-Transfer Coefficient Btu/hr-ft²-°F</u>
Sodium pool, avg. 300-500°F	10	47.14	18.01	2.617	5.1161	<u>100.00</u>	--
Basalt concrete	4	<u>1.20</u>	<u>30.00</u>	0.040	<u>0.63246</u>	<u>160.0</u>	<u>50.00</u>
Stagnant sodium at 210°F	5	<u>50.45</u>	<u>19.13</u>	2.637	<u>5.1354</u>	<u>30.902</u>	<u>258.88</u>
Carbon steel	6	<u>26.00</u>	<u>54.00</u>	0.4815	<u>2.1943</u>	<u>25.620</u>	<u>312.25</u>

*p.B.15**p.B.16, B.17*

The CACECO results for Cell C and Structures 4, 5, 6, and 10 are summarized in Table 3.16. Again, the beginning is taken at the first time step, 0.002 hr. The table lists the energy changes from 0.002 hr to 1.000 hr for the following: (1) Cell C, 380,507 Btu; (2) Structure 10 (sodium pool of Cell C), 380,507 Btu; and (3) Structure 4, 5, and 6, total 380,506 Btu, an equality due to accurate energy balances. Again, these balances are of sufficient importance to justify further checks. For example, using Equation 3.4.5, the following results are obtained:

For the Cell C pool temperatures,

$$\begin{aligned} U_p(t_1) - U_p(t_2) &= (28,548 \text{ lb})(0.3155 \text{ Btu/lb-}^{\circ}\text{F})(499.85^{\circ}\text{F} - 457.78^{\circ}\text{F}) \\ &= (378,920 \text{ Btu}), \text{ which is within 0.4\% of} \\ &\quad \text{the CACECO value listed in Table 3.16.} \end{aligned}$$

For the Structure 10 nodal temperatures,

$$\begin{aligned} U_p(t_1) - U_p(t_2) &= (28,548)(0.3155)(499.40^{\circ}\text{F} - 457.12^{\circ}\text{F}) \\ &\quad (380,811 \text{ Btu}), \text{ which is within 0.1\% of} \\ &\quad \text{the CACECO value listed in Table 3.16.} \end{aligned}$$

Similarly, using Equation 3.4.6, the following results are obtained:

For Structure 4, the concrete floor,

$$\begin{aligned} U_s(t_1) - U_s(t_2) &= (0.63246 \text{ ft})(160.0 \text{ ft}^2)(30.0 \text{ Btu/ft}^3 - ^{\circ}\text{F}) \\ &\quad (100.21^{\circ}\text{F} - 145.05^{\circ}\text{F}) \\ &= (-136,126 \text{ Btu}), \text{ which is within 6.0\% of} \\ &\quad \text{the CACECO value listed in Table 3.16.} \end{aligned}$$

For Structure 5, the sodium floor,

$$\begin{aligned} U_s(t_1) - U_s(t_2) &= (5.1354)(30.902)(19.13)(100.21^{\circ}\text{F} - 144.33^{\circ}\text{F}) \\ &= (-133,940 \text{ Btu}), \text{ which is within 5.9\% of} \\ &\quad \text{the CACECO value listed in Table 3.16.} \end{aligned}$$

TABLE 3.16

CACECO CHECK OF HOT POOL COOLED BY THREE FLOORS

Item	Cell C with Sodium Pool as Heat Structure 10		Floor of 101.2 ft ³ Basalt Concrete, Heat Structure 4		Floor of 158.7 ft ³ Stagnant Sodium Heat Structure 5		Floor of 56.22 ft ³ Carbon Steel Heat Structure 6	
	<u>0.002 hr*</u>	<u>1.000 hr**</u>	<u>0.002****</u>	<u>1.000 hr***</u>	<u>0.002 hr***</u>	<u>1.000 hr****</u>	<u>0.002 hr***</u>	<u>1.000 hr****</u>
Cell temperature, °F (atmosphere and pool)	<u>499.85</u>	<u>457.78</u>						
Atmosphere energy, Btu	<u>16,374</u>	<u>14,941</u>						
Pool energy, Btu	<u>8,670,072</u>	<u>8,290,999</u>						
Total cell energy, Btu	<u>8,686,447</u>	<u>8,305,940</u>						
Cell energy loss, Btu	--	<u>380,507</u>						
Heat-Structure Temperatures								
Active surface, °F	<u>493.40</u>	<u>237.74</u>	<u>102.5</u>	<u>228.6</u>	<u>107.1</u>	<u>228.6</u>	<u>104.9</u>	<u>228.6</u>
Mid plane, °F	<u>499.95</u>	<u>491.81</u>	<u>100.0</u>	<u>132.0</u>	<u>100.0</u>	<u>131.9</u>	<u>100.0</u>	<u>131.9</u>
Adiabatic surface, °F	<u>499.95</u>	<u>555.93</u>	<u>100.0</u>	<u>106.6</u>	<u>100.0</u>	<u>106.0</u>	<u>100.0</u>	<u>106.1</u>
Average, °F	499.40	457.12	100.21	145.05	100.21	144.33	100.21	144.43
Structure sum of heat transfer (energy absorp- tion from start), Btu	+932	+381,439	<u>-313</u>	<u>-128,360</u>	<u>-309</u>	<u>-126,434</u>	<u>-311</u>	<u>-126,645</u>
Structure energy change, Btu		+380,507	--	-128,047	--	-126,125	--	-126,334

* Case 10, pp. 11 & 12

** Case 10, pp. 44 & 45

*** Case 10, p. 10

**** Case 10, p. 43

For Structure 6, the steel floor,

$$\begin{aligned} U_s(t_1) - U_s(t_2) &= (2.1943)(25.620)(54.0)(100.21^\circ\text{F} - 144.43^\circ\text{F}) \\ &= (-134,242 \text{ Btu}), \text{ which is within 6.0\% of} \\ &\text{the CACECO value listed in Table 3.16.} \end{aligned}$$

Again, these checks confirm that the code energy balances are correct.

The CACECO temperatures for the cooling of the Cell C sodium pool heat Structure 10 and the heating of the floor Structures 4, 5 and 6 are plotted on Figure 3.17 and compared to the analytical solution provided by Carslaw and Jaeger⁽⁵⁾ (also shown in Section 3.3 as Figure 3.7) for the solid slab with a step change in surface temperature. For this comparison, the step change in temperature was taken as $V = 200^\circ\text{F}$, which was the planned change for cooling the pool and for heating the floors. The CACECO data are at 1 hr when the Fourier Number is 0.1. The figure illustrates the insidious error that results from having several structures in convection contact with the top or bottom surfaces of the sodium pool: the pool cools too much. In this example, the pool bottom surface cooled to 238°F (below the 300°F midpoint) and the floor surfaces heated to only 229°F ; on Figure 3.17 these temperatures are shown as,

$$\begin{aligned} v_{10}/V &= (500^\circ\text{F} - 238^\circ\text{F})/(200^\circ\text{F}) = 1.31 \text{ for the pool and} \\ v_4/V &= v_5/V = v_6/V = (229^\circ\text{F} - 100^\circ\text{F})/(200^\circ) = 0.63 \text{ for the floors.} \end{aligned}$$

This error arises only for the sodium pool and only for convection boundary conditions at the top or bottom surfaces of this pool. Equation 3.3.4 describes the usual convection boundary condition which relates the thermal conductivity of the structure, K , the temperature gradient at the surface, dT/dn , the heat-transfer coefficient, H , and the temperature drop from the surface to the bulk temperature, $T_s - T_b$:⁽¹⁾

$$-K \, dT/dn = H (T_s - T_b) \quad (3.3.4)$$

HEDL 7904-105.5

FIGURE 3.17. Comparison of CACECO and analytical temperatures in the slab $0 \leq x \leq 1$ with adiabatic boundary at $x = 0$, zero initial temperature and temperature V at $x = 1$. All data are for $\kappa t/l^2 = 0.1$ and the analytical temperatures are from Figure 11, Page 101 of Carslaw and Jaeger.⁽²⁾ The CACECO temperatures are shown by the solid triangles for the concrete slab of Structure 4, by the circles for the sodium slab of Structure 5, by the triangles for the steel slab of Structure 6, and by the bullets for the Cell C sodium pool represented by Structure 10.

This equation is written for the three floors by using subscripts to denote the structure number:

$$-K_4 \, dT_4/dn = H_4 (T_4 - T_{10}) \quad (3.4.7)$$

$$-K_5 \, dT_5/dn = H_5 (T_5 - T_{10}) \quad (3.4.8)$$

$$-K_6 \, dT_6/dn = H_6 (T_6 - T_{10}) \quad (3.4.9)$$

The code extends this boundary equation to the sodium pool in the obvious manner:

$$-K_{10} \, dT_{10}/dn = H_4 (T_{10} - T_4) + H_5 (T_{10} - T_5) + H_6 (T_{10} - T_6) \quad (3.4.10)$$

This pool boundary equation makes the pool temperatures gradient approach the sum of the floor gradients, a result illustrated by the pool and floor gradients shown in Figure 3.17. In particular, the pool gradient will equal the sum when the thermal conductivities are equal ($K_4 = K_5 = K_6 = K_{10}$). The user should note that several structures in convection contact with the top or bottom surfaces of the sodium pool can lead to pool transients that may be in error even though the energy balances are accurate; that is, the pool energy balance may be accurate, but the pool temperature may not be correct.

Overall, in a variety of important situations combining sodium and water pools with heat structures representing roofs, walls, floors and equipment, this Case 10 has shown that the CACECO code provides accurate analyses of pool and heat structure temperatures, their energy transfers, and the energy effects in the cells. Further, the check has confirmed the independence of the heat structures and of the cell pools.

3.5 DEBUG CASES 11 AND 12, RADIATION HEAT TRANSFER

Debug Cases 11 and 12 continue the check of the heat-transfer analyses of the heat structures which model the heat absorption characteristics of the roofs, walls, floors, and equipment of the cells. These two cases concentrate on radiation heat transfer. The cases solve examples provided by Clark, et al⁽⁶⁾ to demonstrate their solution method for the radiation

2

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The two examples provided by Clark, et al,⁽⁶⁾ used the cylinder shown in Figure 3.18. It was small, only about 2.6 inches (6.574 cm) in diameter and 8 inches (20.32 cm) long -- quite minute compared to an LFMBR cell. This cylinder had six walls, A_1 through A_6 . The cylindrical walls A_3 through A_6 were heated by convection and radiation from a 1340°F (1,000 K) heat source. The end wall A_1 was cooled by convection and radiation to a 620°F (600 K) heat sink. The end wall A_2 was cooled by convection and radiation to an 80°F (300 K) heat sink. Heat transfer within the enclosure was solely by radiation. The end wall A_1 consisted of 10 thermal shields, giving this wall the characteristics of an insulated wall; thus, very little heat passed through A_1 . The end wall A_2 had conductance which was ten times the conductances of A_3 through A_6 and which gave this end a characteristic approaching that of a "thin" wall; thus, most of the heat passed through A_2 . The cylindrical walls, A_3 through A_6 were identical except for their relative locations and surface emissivities.

The parameters of Clark's cylinder that were common to the two examples are as follows:

- (a) The conductances of the walls were converted to thermal conductivity for CACECO code input.

<u>Wall</u>	<u>Clark's Conductance</u>	<u>CACECO Input Thermal Conductivity</u>
A_2	4.480 w/K	<u>2.180Btu/hr-ft-°F</u>
A_3 to A_6	0.448	<u>0.04802</u>

p.B.20

- (b) The heat-transfer coefficients on the external surfaces were converted to CACECO code units.

<u>Wall</u>	<u>Clark's Heat-Transfer Coef.</u>	<u>CACECO Input Heat-Transfer Coef.</u>
A_1 and A_2	0.001701 w/cm ² -K	<u>3.00 Btu/hr-ft²-°F</u>
A_3 to A_6	0.002835	<u>5.00</u>

p.B.20

$$\begin{aligned}
 L &= 20.320 \text{ cm} = 8.0 \text{ in.} \\
 r_1 &= 3.098 \text{ cm} = 1.22 \text{ in.} \\
 r_2 &= 3.287 \text{ cm} = 1.29 \text{ in.} \\
 t_2 &= 0.254 \text{ cm} = 0.10 \text{ in.}
 \end{aligned}$$

HEDL 7904-105.4

FIGURE 3.18. Six-Surface Example of Radiation Heat Transfer by Clark, Lammers, Kreplin and Korybalski.⁽⁶⁾

- (c) The 0.05 emissivity for the ten thermal shields of Wall A_1 result in a total interchange area of 0.000832 ft^2 for radiative transfer from from one shield to the next. p.B.20
- (d) The 36 geometrical view factors, F_{ij} , for the internal radiative exchange between the six walls are listed in Table 3.17 as area-view factor products. These view factors were calculated by using the configuration formula and flux algebra formulas provided by Wiebelt.⁽⁷⁾
- (e) The 36 total interchange areas that are used in the analysis of the energy exchange in this gray enclosure are listed in Table 3.18. These were obtained from the emissivities and area-view factor products by using Hottel's method.⁽⁸⁾ Of these 36 areas, only 15 had to be input for the CACECO analysis.

Cases 11 and 12 were planned with the following correspondence between their heat structures and the walls and shields of Clark's examples. Note that a heat structure represented each thermal shield of Wall A_1 .

<u>Heat Structure</u>	<u>Geometry</u>	<u>Clark's Walls and Shields</u>
1	planar	A_1 (Shield 1), internal surface
2	planar	A_2
3, 4, 5, 6	cylindrical	A_3, A_4, A_5, A_6
7 thru 14	planar	A_1 (Shield 2) thru A_1 (Shield 9)
15	planar	A_1 (Shield 10, external surface)

The first example provided by Clark, et al,⁽⁶⁾ had the radiative heat transfer on the external surfaces dominate the convective heat transfer to the extent that the radiative flux was about three times the convective

TABLE 3.17

INTERNAL RADIATION VIEW FACTORS FOR SIX-SURFACE EXAMPLE

Listed is the product: $A_i F_{ij}$,
(the area times the view factor) ft^2

<u>Item</u>	<u>A₁ Wall</u>	<u>A₂ Wall</u>	<u>A₃ Wall</u>	<u>A₄ Wall</u>	<u>A₅ Wall</u>	<u>A₆ Wall</u>
(Area, ft^2)	(0.032 455)	(0.032 455)	(0.106 438)	(0.106 438)	(0.106 438)	(0.106 438)
A ₁	0.0	0.000 721	0.025 186	0.004 708	0.001 320	0.000 519
A ₂	0.000 721	0.0	0.000 519	.001 320	0.004 708	0.025 186
A ₃	0.025 186	0.000 519	0.056 966	0.020 476	0.003 392	0.000 798
A ₄	0.004 708	0.001 320	0.020 476	0.056 066	0.020 476	0.003 392
A ₅	0.001 320	0.004 708	0.003 392	0.020 476	0.056 066	0.020 476
A ₆	0.000 519	0.025 186	0.000 798	0.003 392	0.020 476	0.056 066

TABLE 3.18

INTERNAL TOTAL INTERCHANGE AREAS FOR SIX-SURFACE EXAMPLE

Listed is the product: $A_i F_{ij}$,
(the total interchange area) ft^2

<u>Item</u>	<u>A₁ Wall</u>	<u>A₂ Wall</u>	<u>A₃ Wall</u>	<u>A₄ Wall</u>	<u>A₅ Wall</u>	<u>A₆ Wall</u>
(emissivity)	(0.937)	(0.518)	(0.426)	(0.375)	(0.355)	(0.336)
A ₁	0.005 130	<u>0.000 849</u>	<u>0.015 704</u>	<u>0.005 270</u>	<u>0.002 251</u>	<u>0.001 204</u>
A ₂	0.000 849	0.002 149	<u>0.000 698</u>	<u>0.001 490</u>	<u>0.003 419</u>	<u>0.008 206</u>
A ₃	0.015 704	0.000 698	0.016 773	<u>0.008 015</u>	<u>0.002 880</u>	<u>0.001 272</u>
A ₄	0.005 270	0.001 490	0.008 015	0.014 559	<u>0.007 557</u>	<u>0.003 023</u>
A ₅	0.002 251	0.003 419	0.002 880	0.007 557	0.013 910	<u>0.007 768</u>
A ₆	0.001 204	0.008 206	0.001 272	0.003 023	0.007 768	0.014 290

The total interchange areas underlined were input by the Card series 400001 for the CACECO code analyses.

p.B.20

flux. The second example had the reverse situation: the radiative flux was only about half the convective flux. The radiative heat transfer was set by the emissivities used on the external surfaces. These emissivities and the associated total interchange areas are listed below for the two examples.

TABLE 3.19

EXTERNAL TOTAL INTERCHANGE AREAS FOR BOTH EXAMPLES

Wall External Surface	First Example		Second Example	
	Emissivity	Total Interchange* Area, ft ²	Emissivity	Total Interchange** Area, ft ²
A ₁	0.937	<u>0.030 41</u>	0.050	<u>0.001 62</u>
A ₂	0.518	<u>0.016 81</u>	0.050	<u>0.001 62</u>
A ₃	0.426	<u>0.048 11</u>	0.050	<u>0.005 65</u>
A ₄	0.375	<u>0.042 35</u>	0.050	<u>0.005 65</u>
A ₅	0.355	<u>0.040 09</u>	0.050	<u>0.005 65</u>
A ₆	0.336	<u>0.037 94</u>	0.050	<u>0.005 65</u>

*p. B.20

**p. B.29

The steady-state solutions for these two examples were provided by Clark, et al, to illustrate the power of their analysis method. The CACECO code calculates a steady-state solution for the cell conditions and for the heat-structure temperatures prior to beginning the transient analysis. The purpose of this steady-state solution is to provide the appropriate initial conditions for the transient. Usually the transient results are the main interest of the CACECO analysis; but, for these examples the steady-state solution is the main interest.

The CACECO code steady-state analysis of the heat-structure temperatures is done in 2 to 6 iterations to accommodate (a) temperature-dependent

convection boundaries and (b) radiative heat exchanges. The code uses the initial surface temperatures provided between Card 500000 and Card 600000 to begin the iteration process. The code sums the surface temperatures of all of the heat structures and stops this iteration process when this sum changes by 1°F or less or on the 6th iteration, whichever occurs first. The code user can use the iterative results of one run as the initial temperatures of the next run in order to increase the total number of iterations and thereby improve the analysis of the steady-state conditions.

Debug Case 11 was used to illustrate the results obtained by successive runs, with each run using the surface temperatures obtained by the preceding run. The results of 12 runs with a total of 72 iterations are listed in Table 3.20. The first iteration began with the sink-source temperatures: 620°F for Wall A_1 , 80°F for Wall A_2 , and 1340°F for Walls A_3 through A_6 . Only a few runs were needed to obtain surface temperatures for Walls A_2 through A_6 that differed by 1°F or less from the values at the end of the 12th run. However, the thermal shields of Wall A_1 did not reach converged values even by the 12th run. The code user can monitor the temperatures of selected heat structures when one or a few are of main importance; but, more likely during a successive run-iterative process the user will monitor the sum of surface temperatures listed by the code. These sums are listed in Table 3.20, and the first run changed the sums by about 5000°F , the fifth run by about 500°F and the tenth run by about 50°F . Obviously this iteration process converges, and the user must decide when the results are good enough for his purposes.

p.B.18

The surface temperatures of Debug Case 11 are compared to the results provided by Clark, et al, in Table 3.20. The CACECO temperatures of Walls A_2 through A_6 differed from Clark's by an average of 0.9°F at the end of the second run and by an average of 0.6°F at the end of the twelfth run. The CACECO temperatures of Wall A_1 are different from Clark's, and this difference must be due to inconsistency in Clark's data. The heat exchanges of Debug Case 11 are compared to those provided by Clark, et al, in Table 3.21.

TABLE 3.20
CHECK CASE 11 TEMPERATURES

		Listed is the Temperature, °F														First Example Clark et al(6)	Difference
Temperature Note 1	Note 2	Run No Iteration No.	0	1	2	3	4	5	6	7	8	9	10	11	12		
			0	6	12	18	24	30	36	42	48	54	60	66	72		
T _{1i}	T _{1,1}		620.3	1268.0	1279.3	1281.0	1281.7	1282.1	1282.3	1282.8	1282.7	1282.7	<u>1282.8</u>	<u>1282.8</u>	<u>1282.8</u>	1285.4	2.6
T _{2i}	T _{2,1}		80.3	836.9	841.2	841.8	841.9	842.0	842.1	842.3	<u>842.2</u>	<u>842.2</u>	<u>842.2</u>	<u>842.2</u>	<u>842.2</u>	840.8	1.4
T _{2e}	T _{2,5}		80.3	819.6	823.7	824.3	824.4	824.5	824.6	824.8	<u>824.7</u>	<u>824.7</u>	<u>824.7</u>	<u>824.7</u>	<u>824.7</u>	823.6	1.1
T _{3i}	T _{3,1}		1340.3	1296.5	1299.3	1300.0	1300.2	1300.4	1300.5	1300.8	<u>1300.6</u>	<u>1300.6</u>	<u>1300.6</u>	<u>1300.6</u>	<u>1300.6</u>	1301.3	0.7
T _{3e}	T _{3,7}		1340.3	1329.1	1329.8	1330.0	1330.1	1330.1	1330.1	<u>1330.2</u>	<u>1330.2</u>	<u>1330.2</u>	<u>1330.2</u>	<u>1330.2</u>	<u>1330.2</u>	1330.2	0.0
T _{4i}	T _{4,1}		1340.3	1290.1	1294.0	1294.5	1294.7	1294.8	1294.9	1295.1	<u>1295.0</u>	<u>1295.0</u>	<u>1295.0</u>	<u>1295.0</u>	<u>1295.0</u>	1296.2	1.2
T _{4e}	T _{4,7}		1340.3	1326.5	1327.6	1327.7	1327.8	1327.8	1327.8	1327.9	1327.8	1327.8	<u>1327.9</u>	<u>1327.9</u>	<u>1327.9</u>	1327.7	0.2
T _{5i}	T _{5,1}		1340.3	1273.7	1276.8	1277.2	1277.3	1277.4	1277.4	1277.6	<u>1277.5</u>	<u>1277.5</u>	<u>1277.5</u>	<u>1277.5</u>	<u>1277.5</u>	1277.7	0.2
T _{5e}	T _{5,7}		1340.3	1321.4	1322.3	1322.4	1322.4	<u>1322.5</u>	<u>1322.5</u>	<u>1322.5</u>	<u>1322.5</u>	<u>1322.5</u>	<u>1322.5</u>	<u>1322.5</u>	<u>1322.5</u>	1322.0	0.5
T _{6i}	T _{6,1}		1340.3	1239.8	1242.3	1242.6	1242.7	1242.8	1242.8	1242.9	1242.8	1242.8	1242.8	1242.8	<u>1242.9</u>	1242.4	0.5
T _{6e}	T _{6,7}		1340.3	1310.8	1311.6	1311.7	1311.7	1311.7	1311.7	1311.8	<u>1311.7</u>	<u>1311.7</u>	<u>1311.7</u>	<u>1311.7</u>	<u>1311.7</u>	1311.5	0.2
T _{s2}	T _{7,1}		620.3	1160	1193	1210	1220	1226	1231	1234	1236	1237	1238	1239	1239	-	
T _{s3}	T _{8,1}		620.3	939	1068	1116	1143	1159	1170	1178	1183	1186	1189	1190	1191	-	
T _{s4}	T _{9,1}		620.3	896	1000	1051	1082	1102	1115	1125	1131	1135	1138	1139	1141	-	
T _{s5}	T _{10,1}		620.3	684	850	938	989	1022	1043	1058	1068	1074	1078	1081	1083	-	
T _{s6}	T _{11,1}		620.3	682	814	890	936	966	986	999	1008	1013	1017	1020	1021	-	
T _{s7}	T _{12,1}		620.3	620	696	781	839	897	902	919	930	938	943	946	948	-	
T _{s8}	T _{13,1}		620.3	620	685	747	788	815	833	845	853	858	862	864	866	-	
T _{s9}	T _{14,1}		620.3	620	633	667	697	719	733	744	750	755	758	760	762	-	
T _{1e}	T _{15,3}		620.3	620.3	620.7	621.6	622.2	622.7	623.0	623.3	623.4	623.6	623.6	<u>623.7</u>	<u>623.7</u>	646.6	22.9
Sum of Surface Temp.			<u>23,290</u>		<u>29,751</u>		<u>31,270</u>		<u>31,914</u>		<u>32,207</u>		<u>32,332</u>		<u>32,391</u>	Case 11, vp. 13,14,15.	
				<u>28,264</u>		<u>30,678</u>		<u>31,658</u>		<u>32,092</u>		<u>32,281</u>		<u>32,367</u>			
Change in Sum of Surface Temp.			-	4,974	1,487	927	592	388	256	178	115	74	51	35	24		

The temperatures underlined are the same as that at the end of Run No. 12.

- Notes: 1. Wall or shield by Clark: first subscript denotes wall number (1, 2, etc.) or shield(s); the second subscript denotes internal (i) or external (e) surface or shield number (2, 3, etc.) of Wall A₁. Note the identities: T_{1i} = T_{5i}, T_{1e} = T_{5e}.
2. CACECO heat structures: first subscript denotes structure number (1, 2, etc.) and the second subscript denotes node number (1, 3, 5 or 7).

TABLE 3.21

CHECK CASE 11 HEAT EXCHANGES

Listed is the Heat Exchange, Btu/hr

Wall	Run No. 2	Run No. 12	First Example Clark, et al ⁽⁶⁾	Difference
A ₁	-3.39	-1.28	-1.000	(22%)
A ₂	-148.1	-148.4	-146.82	(1.0%)
A ₃	26.0	25.1	24.64	(1.8%)
A ₄	28.3	27.9	27.31	(2.2%)
A ₅	38.5	38.2	38.07	(3.0%)
A ₆	58.7	58.5	58.73	(0.4%)

The CACECO heat exchanges of Walls A₂ through A₆ differed from Clark's by an average of 2.8% at the end of the second run and by an average of 1.7% at the end of the twelfth run. Again, the CACECO heat exchange of Wall A₁ is different from Clark's, and this difference must be due to inconsistency in Clark's data. This inconsistency is shown below by the calculation of the convective and radiative heat transfers from Wall A₁ to the 600 K sink. The cgs units of Clark are used.

$$\begin{aligned}
 \text{Convective: } q &= h A (T_1 - T_s) \\
 &= (0.001701 \text{ w/cm}^2\text{-K})(30.2 \text{ cm}^2)(614.6-600\text{K}) \\
 &= 0.75 \text{ w}
 \end{aligned}$$

$$\begin{aligned}
 \text{Radiative: } q &= A (T_1^4 - T_s^4) \\
 &= (5.67 \times 10^{-12} \text{ w/cm}^2\text{-K}^4)(0.336)(30.2 \text{ cm}^2) \\
 &\quad \times (614.6^4 - 600.0^4\text{K}^4) \\
 &= 0.75 \text{ w}
 \end{aligned}$$

Clark, et al, had listed the heat transfer through Wall A_1 as 0.29 w, considerably less than either the convective (0.75 w) or radiative (0.75 w) heat transfer obtained by calculating from their data.

p.B.27

Debug case 12 was used to illustrate the results obtained by an outside estimate of the initial temperatures in order to speed the iteration process. The surface temperatures of this case are compared to those of the second example provided by Clark, et al, in Table 3.22. There are a number of methods outside the CACECO code to use to obtain these initial temperatures. In this case, the first run began with the following sink-source temperatures: 620°F for Wall A_1 , 80°F for Wall A_2 , and 1340°F for Walls A_3 through A_6 . This first run obtained 1255°F for Wall A_1 internal temperature, which is the temperature of Shield 1 of this wall. The author then split the temperature difference, 1255°F - 620°F, among the other nine shields first uniformly and then nonuniformly by taking into account the $1/T^3$ variation in temperature drop due to radiative heat transfer between shields. The results of these hand calculations were used to begin the second run. The results of this second run are compared to those provided by Clark, et al, in Table 3.22. The CACECO temperatures of Walls A_2 through A_6 differed from Clark's by an average of 1.2°F at the end of this run; again, wall A_1 is different.

Overall, these comparisons with the results obtained by Clark, et al, confirm the accuracy of the radiative heat transfer analyses provided by the CACECO code.

TABLE 3.22

CHECK CASE 12 TEMPERATURES

Listed is the temperature, °F

Temperature Note 1	Note 2	Run No. Iteration No.	0 0	1 6	- 6	2 12	Second Example Clark et al(6)	Difference
T _{1i}	T _{1,1}		620.3	1255.2	1255.2	1277.0		
T _{2i}	T _{2,1}		80.3	998.1		1011.6		
T _{2e}	T _{2,5}		80.3	986.3		999.6	1001.6	2.0
T _{3i}	T _{3,1}		1340.3	1283.6		1291.5		
T _{3e}	T _{3,7}		1340.3	1310.8		1315.0	1316.6	1.6
T _{4i}	T _{4,1}		1340.3	1277.6		1287.3		
T _{4e}	T _{4,7}		1340.3	1307.7		1312.8	1313.7	0.9
T _{5i}	T _{5,1}		1340.3	1265.0		1273.2		
T _{5e}	T _{5,7}		1340.3	1301.1		1305.4	1304.3	1.1
T _{6i}	T _{6,1}		1340.3	1238.2		1245.9		
T _{6e}	T _{6,7}		1340.3	1287.1		1291.1	1291.7	0.6
T _{s2}	T _{7,1}		620.3	1152	1217.	1232.		
T _{s3}	T _{8,1}		620.3	926	1177.	1184.		
T _{s4}	T _{9,1}		620.3	893	1134.	1138.		
T _{s5}	T _{10,1}		620.3	680	1086.	1086.		
T _{s6}	T _{11,1}		620.3	682	1034.	1032.		
T _{s7}	T _{12,1}		620.3	620	976.	964.		
T _{s8}	T _{13,1}		620.3	620	909.	886.		
T _{s9}	T _{14,1}		620.3	620	831.	779.		
T _{1e}	T _{15,3}		620.3	620	735	632.7	638.2	50.5

Sum of
Surface temp.23,29028,39332,95232,757Case 12,
pp. 13, 14, 15Notes

1. Wall or shield by Clark: first subscript denotes wall number (1, 2, etc.) or shield(s); the second subscript denotes internal (i) or external (e) surface or shield number (2, 3, etc.) of Wall A₁. Note the identities:

$$T_{1i} = T_{s1}, T_{1e} = T_{s10}.$$

2. CACECO heat structures: first subscript denotes structure number (1, 2, etc.) and the second subscript denotes node number (1, 3, 5, or 7).

3.6 DEBUG CASES 13, 14 AND 15, CONCRETE HEAT STRUCTURES

Debug Cases 13, 14 and 15 continue the check of the heat-conduction analyses of the heat structures which model the heat absorption characteristics of the roofs, walls and floor of the cells. These three cases concentrate on concrete, the releases of water and carbon dioxide that occur when concrete is heated the first time, and the material, energy and chemical reaction effects as the water and carbon dioxide enter cells filled with air or with a sodium pool. The cases solve examples which were invented to demonstrate the capabilities of the code. The capabilities are important because concrete is the universal material of construction of LMFBF facilities.

These cases continue the check of the many input data cards which are used to describe the heat structures and their heat transfer -- cards which have been checked by Debug Cases 9 through 12. The present cases also check the input data cards which are used to describe the concrete properties, and these are summarized below.

<u>Input Data Description</u>	<u>Card Numbers</u>
Concrete additional heat capacity	Card series 2201
Concrete thermal conductivity	Card series 2301
Concrete water release	Card series 2501
Structures that release concrete water	Card series 2601
Concrete carbon dioxide release	Card series 2701
Structures that release concrete carbon dioxide	Card series 2801
Heat structure material data	Card series 300001

The concrete used in these three cases was invented to make the code check easy; its properties only approximate those of real concrete. This invented concrete had limestone aggregate because the other aggregates of interest to the author, basalt and magnetite, do not release significant quantities of carbon dioxide when heated. However, all kinds of concrete

release water when heated because water is used to make concrete. The water release for the concrete of these cases, defined by Card Series 2501, was set so that no water was released as the concrete heated to 200°F, then a linear release up to the maximum available of 9.0 lb/ft³ (1b of water/ft³ of concrete) at 700°F. The carbon dioxide release, defined by Card Series 2701, was set to zero as the concrete heated to 1200°F, and then to a linear release up to the maximum available of 22.0 lb/ft³ (1b of carbon dioxide/ft³ of concrete) at 1700°F. These water and carbon dioxide releases are graphed in Figure 3.19 at the top.

p.B.33

p.B.33

The concrete was assumed to have a density of $\rho = 150 \text{ lb/ft}^3$ and a constant (for both heating and cooling) heat capacity of $C = 0.26 \text{ Btu/lb}^\circ\text{F}$. The volumetric heat capacity used by the code was then $\rho C = \underline{39 \text{ Btu/ft}^3\text{-}^\circ\text{F}}$, and this value was input by the Card Series 300001. Additional heat energy must be absorbed by concrete in order to release the water and carbon dioxide, and the CACECO code accounts for this heat energy by an additional, temperature-dependent heat capacity which is added to the constant heat capacity of the material. That is, the code adds the heat capacity input on Card Series 2201 to the heat capacity input by Card Series 300001 when the material is identified as concrete and the structure temperatures are increasing for the first time. For water, this additional energy was approximated by the latent heat of 1162 Btu/lb of water. For carbon dioxide, this additional energy was approximated by the chemical reaction heat of calcination of 1676 Btu/lb of carbon dioxide. The values of additional heat capacity used by the code are calculated by the user from the material released, $R_2 - R_1$, and its energy effect, Q , over the temperature range, $T_2 - T_1$, using the following equation:

p.B.35

$$\rho C = (R_2 - R_1)Q / (T_2 - T_1) \quad (3.6.1)$$

For the water release from 200° to 700°F,

$$\begin{aligned} &= (9.0 \text{ lb/ft}^3 - 0.0)(1162 \text{ Btu/lb}) / (700^\circ\text{F} - 200^\circ\text{F}) \\ &= (\underline{20.92 \text{ Btu/ft}^3 - ^\circ\text{F}}) \end{aligned}$$

p.B.33

FIGURE 3.19. Limestone Concrete Properties Used in Debug Cases 13 through 15.

For the carbon dioxide release from 1200 to 1700°F:

$$\begin{aligned}\rho C &= (22.0 \text{ lb/ft}^3 - 0.0)(1676 \text{ Btu/lb})/(1700^\circ\text{F} - 1200^\circ\text{F}) \\ &= \underline{(73.94 \text{ Btu/ft}^3 - ^\circ\text{F})}\end{aligned}$$

p.B.33

The additional heat capacity effects for the water and carbon dioxide releases are graphed in Figure 3.19. The code would use the following heat capacities if the concrete were subjected to the following sequence of transients:

<u>Transient</u>	<u>Concrete Heat Capacity</u>
Heat 76°F to 200°F	39 Btu/ft ³ -°F
Heat 200°F to 700°F	59.92
Heat 700°F to 1200°F	39.0
Heat 1200°F to 1700°F	112.94
Heat 1700°F to 2000°F	39.0
Cool 2000°F to 100°F	39.0
Reheat 100°F to 200°F	39.0
Reheat 200°F to 1700°F	39.0

The thermal conductivity of concrete is input by Card Series 2301 as temperature-dependent thermal conductivity. In comparison, the usual materials for heat structures are assumed to have constant values for thermal conductivity (and volumetric heat capacity), which are input by Card Series 300001. However, the code uses the thermal conductivity input on Card Series 2301 instead of the value input by Card Series 300001 when the material is identified as concrete. The concrete for these cases was assumed to have thermal conductivity of $K = \underline{0.7 \text{ Btu/hr-ft-}^\circ\text{F}}$ up to $\underline{800^\circ\text{F}}$, then a linear decrease to the minimum value of $K = \underline{0.5 \text{ Btu/hr-ft-}^\circ\text{F}}$ at $\underline{1100^\circ\text{F}}$. This temperature dependence is shown in Figure 3.19 at the bottom.

p.B.33

p.B.33,
B.34

These cases were planned so that water and carbon dioxide would be released from heat structures of the different geometries: slab (planar), cylindrical and spherical. The structures were sized so that their Fourier Number would equal $t/l^2 = 0.1$ at $t = 10$ hours. Thus, the thickness of the slab and the radius of the cylinder and sphere structures were $l = 1.08084$ ft for the structures with water and $l = 0.66537$ ft for the structures with carbon dioxide. Also, all heat structures had the same volume, 20 ft^3 .

Further, these cases were planned so that the concrete structures would demonstrate water and carbon dioxide releases by heating transients similar to those already checked by Debug Case 9. The transients used are due to a step change in surface temperature and are shown in Figures 3.7, 3.9 and 3.11 for the slab, cylindrical and spherical structures, respectively. The plan was that concrete Structures 1, 2 and 3 would release water as they heated from 200°F up towards 700°F and that Structures 4, 5, and 6 would release carbon dioxide as they heated from 1200°F up towards 1700°F . These six structures are present in Cases 13, 14 and 15.

The CACECO temperatures for Structures 1 to 6 are compared with the analytical temperatures graphed by Carslaw and Jaeger⁽²⁾ in Figure 3.20, 3.21 and 3.22 for the slab, cylindrical and spherical geometries, respectively. Excellent agreement is shown by this comparison of temperatures at the Fourier Number $\kappa t/l^2 = 0.1$ which occurs in these structures at $t = 10$ hr. This excellent agreement proves that the CACECO code can properly use the temperature-dependent thermal conductivity data input in Card Series 2301 and can sum the temperature-dependent additional heat capacity data input in Card Series 2201 with the constant heat capacity data input in Card Series 300001.

The code assumes that water and carbon dioxide are released from structures which are heated by the boundary condition of temperature node No. 1, which is the boundary condition inside the structures of cylindrical and spherical geometry. This boundary condition for node No. 1 is printed in CACECO output on the left-hand side and is visualized by the code author

FIGURE 3.20. Comparison of CACECO and analytical temperatures in the slab $0 < x < 1$ with adiabatic boundary at $x = 0$, zero initial temperature and temperature V at $x = 1$. The numbers on the curves are the values of kt/l^2 . The CACECO temperatures are shown by the bullets for Structure 1 with its water release and by the circles for Structure 4 with its carbon dioxide release. Analytical temperatures are from Figure 11, Page 101 of Carslaw and Jaeger.⁽²⁾

FIGURE 3.21. Comparison of CACECO and analytical temperatures in the cylinder of radius a with zero initial temperature and surface temperature V . The numbers on the curves are the values of $\kappa t/a^2$. The CACECO temperatures are shown by the bullets for Structure 2 with its water release and by the circles for Structure 5 with its carbon dioxide release. Analytical temperatures are from Figure 24, Page 200 of Carslaw and Jaeger.⁽²⁾

FIGURE 3.22. Comparison of CACECO and analytical temperatures in the sphere of radius a with zero initial temperature and surface temperature V . The numbers on the curves are the values of $\kappa t/a^2$. The CACECO temperatures are shown by the bullets for Structure 3 with its water release and by the circles for Structure 6 with its carbon dioxide release. Analytical temperatures are from Figure 29, Page 234 of Carslaw and Jaeger.⁽²⁾

as the left surface for all nonpool structures. The code uses this assumption of structure heating from the left-hand side to determine the energy carried by each (time step) increment of water and carbon dioxide release: each incremental release has energy at the temperature of node No. 1 as if it had heated (or cooled) in passing through the structure from its actual release location to the left-hand surface. For these debug cases, the incremental water release would have the energy of 1072.06 Btu/lb if the node No. 1 temperature were 200°F, and 1249.51 Btu/lb if it were 700°F; the incremental carbon dioxide release would have the energy of 243.75 Btu/lb if the node No. 1 temperature were 1200°F, and 370.05 Btu/lb if it were 1700°F. With each heat structure having a 20 ft³ volume, these debug cases would have the following maximum values of material releases and of energy effects:

Structures with water release:

Water release: $R_{H_2O} = (20 \text{ ft}^3)(9.0 \text{ lb/ft}^3) = 180 \text{ lb water}$

Energy absorbed
by structure: $U_S(700^\circ\text{F}) - U_S(200^\circ\text{F}) = (20 \text{ ft}^3)(59.92 \text{ Btu/ft}^3\text{-}^\circ\text{F})$
 $\times (700^\circ\text{F} - 200^\circ\text{F})$
 $= 599,200 \text{ Btu}$

Energy carried by
water release to
cell destination: $U_{H_2O}R_{H_2O} = (1249.51 \text{ Btu/lb})(180 \text{ lb})$
 $= 224,912 \text{ Btu}$

Structures with carbon dioxide release:

Carbon dioxide
release: $R_{CO_2} = (20 \text{ ft}^3)(22.0 \text{ lb/ft}^3) = 440 \text{ lb carbon dioxide}$

Energy absorbed
by structure:

$$\begin{aligned} U_S(1700^{\circ}\text{F}) - U_S(1200^{\circ}\text{F}) &= (20 \text{ ft}^3)(112.94 \text{ btu/ft}^3\text{-}^{\circ}\text{F}) \\ &\quad *(1700^{\circ}\text{F} - 1200^{\circ}\text{F}) \\ &= 1,129,400 \text{ Btu} \end{aligned}$$

Energy carried by
carbon dioxide release

$$\begin{aligned} \text{to cell destination: } U_{\text{CO}_2} R_{\text{CO}_2} &= (370.05 \text{ Btu/lb})(440 \text{ lb}) \\ &= 162,822 \text{ Btu} \end{aligned}$$

The CACECO code calculates the water and carbon dioxide release from each structure by using the temperature distribution within the structure. This calculation is not time dependent except as the temperatures are time dependent and, in particular, the release will not increase unless the temperatures increase. The code divides the structure into volume increments, each increment being the volume between successive temperature node locations. Subroutine CWRF calculates the water release of a structure by the following steps:

1. At each temperature node, interpolate the temperature-dependent water release from the table input by Card Series 2501.
2. Check each volume increment for concrete as identified by Card Series 2201, skip over nonconcrete increments.
3. Average the water release across each concrete volume increment and calculate the incremental release for the increment.
4. Sum the incremental releases for the whole structure.

Subroutine C02F calculates the carbon dioxide release of a structure by these same four steps.

In the present case, the water and carbon dioxide releases are linear with temperature and are proportional to the change in sensible energy of

each structure which, in turn, is equal to the heat energy transferred to each structure. The CACECO code calculates the heat energy transferred by the integration of the heat-transfer rates over time. A comparison of (a) change in sensible energy and (b) heat energy transferred was made in Section 3.3 and shown for Debug Case 9 in Table 3.8. A similar comparison, including water and carbon dioxide releases, is shown for Debug Case 13 in Table 3.23. As noted previously, the hand calculation of the volume integral of the analytical solutions does not provide high precision because of the author's difficulty in reading values of temperature from the graphs. Nevertheless, the comparisons shown in Table 3.23 substantiate the accuracy of the CACECO results for material releases and energy transferred.

These cases were planned so that the maximum material release and associated energy effect from each structure would heat each cell 100°F. The planning analyses are outlined below.

180-lb Water Release at 700°F into Air-Filled Cell

p.B.33 The input data cards (for example, Cards 2 and 3 for Cell A) define this cell as having 26,326 ft³ of air (21% oxygen) with 100% relative humidity (for water vapor) at 100°F and 14.7 psia. The initial conditions of this cell are as follows:

Atmosphere mass:

*Case 13,
p.12*

$$M_a = (\underline{75.38 \text{ lb H}_2\text{O}} + \underline{1333.80 \text{ lb N}_2} + \underline{404.97 \text{ lb O}_2})$$

Atmosphere energy:

*Case 13,
p.12*

$$U_a = (\underline{107,906 \text{ Btu}})$$

The concrete water release transient requires integration of the following portions of the mass and energy differential equations for the cell.

TABLE 3.23

CHECK CASE 13 MATERIAL RELEASES AND ENERGY TRANSFERS(Fourier Number $\kappa t/l^2 = 0.1$ at $t = 10$ hr)

<u>Item</u>	<u>CACECO Results*</u>	<u>Maximum Value</u>	<u>Fraction</u>
Slab Geometry: analytical solution in Figure 11 of Carslaw and Jaeger, Volume integral of temperature			0.359
Structure 1:			
Water release, lb	<u>62.8</u>	180.	0.349
Energy transferred, Btu	<u>-203,860</u>	-599,200	0.340
Structure 4:			
Carbon dioxide release, lb	<u>153.0</u>	440.	0.348
Energy transferred, Btu	<u>-383,969</u>	-1,129,400	0.340
-----			-----
Cylindrical Geometry: analytical solution in Figure 24 of Carslaw and Jaeger, Volume integral of temperature			0.613
Structure 2:			
Water release, lb	<u>106.6</u>	180.	0.592
Energy transferred, Btu	<u>-345,673</u>	-599,200	0.577
Structure 5:			
Carbon dioxide release, lb	<u>259.9</u>	440.	0.591
Energy transferred, Btu	<u>-651,959</u>	-1,129,400	0.577
-----			-----
Spherical Geometry: analytical solution in Figure 29 of Carslaw and Jaeger, Volume integral of temperature			0.774
Structure 3:			
Water release, lb	<u>136.0</u>	180.	0.756
Energy transferred, Btu	<u>-438,732</u>	-599,200	0.732
Structure 6:			
Carbon dioxide release, lb	<u>331.7</u>	440.	0.754
Energy transferred, Btu	<u>-828,646</u>	-1,129,400	0.734

* Case 13, pp. 27, 28

Atmosphere mass:

$$dM_a/dt = \sum_N R_{H_2O} \quad (3.6.2)$$

Atmosphere energy:

$$dU_a/dt = \sum_N U_{H_2O} R_{H_2O} \quad (3.6.3)$$

With the maximum 180-lb water release and associated energy already cited, the final conditions of this cell would be as follows:

Atmosphere mass:

$$M_a = (255.38 \text{ lb } H_2O + 1333.80 \text{ lb } N_2 + 404.97 \text{ lb } O_2)$$

Atmosphere energy:

$$U_a = (332,818 \text{ Btu})$$

Subroutine EMVBAL would iterate to find the cell temperature at 200°F; that is, the water release would heat the cell from 100°F to 200°F.

180-lb Water Release at 700°F into Inerted Cell with Sodium Pool

p.B.33 The input data cards (for example, Cards 4 and 5 for Cell B) define this cell as having 4504 ft³ of nitrogen with no oxygen or water vapor at 500°F and 10.835 psia, and with a 46,989 lb sodium pool at 500°F. The initial conditions of this cell are as follows:

Atmosphere mass:

$$M_a = (\underline{5.2 \times 10^{-4} \text{ lb}} \text{ Na} + \underline{132.76 \text{ lb}} \text{ N}_2)$$

Case 13,
p.15

Sodium pool mass:

$$M_p = (46,989) \text{ lb Na}$$

Case 13, p. 13

Atmosphere energy:

$$U_a = (11,810 \text{ Btu})$$

Pool Energy:

$$U_p = (14,273,000 \text{ Btu})$$

Input to the CACECO code must specify the destination of this concrete water release and, in particular with a sodium pool, whether the release enters the atmosphere or the pool of the cell. The chemical reaction of sodium and water is

but, sodium vapor reacts in the atmosphere and sodium liquid reacts in the pool. In the atmosphere, the heat of this chemical reaction is 3400 Btu/lb Na vapor and in the pool, 1600 Btu/lb Na liquid. In these cases, Card Series 2601 specifies that the water release enters the sodium pool. The concrete water release transient requires integration of the following portions of the mass and energy differential equations for the cell:

Atmosphere mass:

$$dM_a/dt = R_{\text{Na}_2\text{O}} + R_{\text{H}_2} + R_{\text{NaH}} + B \quad (3.6.5)$$

Sodium pool mass:

$$dM_p/dt = \sum_N R_{\text{H}_2\text{O}} - R_{\text{Na} + \text{H}_2\text{O}} - R_{\text{Na} + \text{H}_2} - B \quad (3.6.6)$$

Atmosphere energy:

$$dU_a/dt = U_g B \quad (3.6.7)$$

Pool energy:

$$dU_p/dt = \sum_N U_{H_2} R_{H_2O} + Q_{Na + H_2O} + Q_{Na + H_2} - U_g B \quad (3.6.8)$$

The new features of this case are the chemical reactions (1) between the pool sodium and water vapor to generate hydrogen and (2) between the pool sodium and hydrogen to generate sodium hydride. The first chemical reaction is

with the attendant stoichiometric relation of

$$\begin{aligned} &2 (22.991 \text{ lb Na/atom}) + 18.016 \text{ lb H}_2\text{O/mole} \\ &= (61.982 \text{ lb Na}_2\text{O/mole}) + (2.016 \text{ lb H}_2\text{/mole}) \end{aligned}$$

For this case, the stoichiometric relation has 459.41 lb sodium reacting with the maximum 180-lb water release to form 619.27 lb sodium oxide and 20.142 lb hydrogen. The second chemical reaction is

with the attendant stoichiometric relation of

$$2 (22.991 \text{ lb Na/atom}) + (2.016 \text{ lb H}_2\text{/mole}) = 2 (23.999 \text{ lb NaH/mole})$$

Again for this case, if all of the hydrogen reacted, the stoichiometric relation would have another 459.41 lb sodium reacting with the 20.142 lb hydrogen to form 479.55 lb sodium hydride. The code considers this hydride reaction to be an equilibrium process that can proceed either way, towards sodium hydride or towards sodium and hydrogen, depending on conditions.

The saturation properties for sodium hydride at 600°F are

Hydrogen pressure: $P_{H_2} = \underline{0.3919 \text{ psia}}$

p.A.6

Hydride solubility: $S_{NaH} = \underline{0.0005117 \text{ lb NaH/lb Na}}$

Heat of formation: $Q_{NaH} = \underline{1053.52 \text{ Btu/lb-NaH}}$

Assuming as a first estimate that all the hydrogen reacts to form hydride, the integration Equation 3.6.6 would be

$$\begin{aligned} M'_p &= M_p + \sum_N R_{H_2O} - R_{Na + H_2O} - R_{Na + H_2} - B \\ &= (46,989 \text{ lb Na}) + (180.0 \text{ lb } H_2O \text{ release}) \\ &\quad - (459.41 \text{ lb Na reacts with this } H_2O) \\ &\quad - (459.41 \text{ lb Na reacts with the } H_2) \\ &\quad - (0 \text{ lb Na evaporation}) \\ &= (46,070.2 \text{ lb } N_a \text{ in pool}) \end{aligned} \quad (3.6.10)$$

At 600°F, this pool mass occupies 842.2 ft³ of the 4504 ft³ cell volume leaving hydrogen and nitrogen in the atmosphere volume of 3661.8 ft³. At the hydrogen saturation pressure of 0.3819 psia, there would be 0.248 lb hydrogen in the atmosphere. With 20.142 lb hydrogen formed by the sodium-water reaction and 0.248 lb in the atmosphere, 19,894 lb must have reacted with 453.75 lb sodium to form 473.65 lb sodium hydride. The second estimate uses this 453.75 lb sodium in Equation 3.6.10 to have 46,075.8 lb sodium in the pool (which occupies 842.3 ft³ of the cell) which leaves an atmosphere volume with 0.248 lb of hydrogen, the same quantity as obtained in the first estimate. This rapid convergence is typical of the sodium hydride equilibrium analysis. The amount of sodium hydride in solution would be

$$\begin{aligned} M_p S_{NaH} &= (46,076 \text{ lb Na})(0.0005117 \text{ lb NaH/lb Na}) \\ &= 23.6 \text{ lb NaH.} \end{aligned}$$

This means that 450.1 lb sodium hydride would precipitate from the sodium pool. The energy effects of this water release and chemical reactions in the cell are most easily solved by adding Equations 3.6.7 and 3.6.8 and then integrating:

$$\begin{aligned}
 U'_a + U'_p &= U_a + U_p + \sum_N U_{H_2O} R_{H_2O} + Q_{Na + H_2O} + Q_{Na + H_2} \quad (3.6.11) \\
 &= (11,810 \text{ Btu in atmosphere}) + (14,273,000 \text{ Btu in pool}) \\
 &\quad + (224,912 \text{ Btu in water release at } 700^\circ\text{F}) \\
 &\quad + (459.41 \text{ lb Na reacted with water})(1600 \text{ Btu/lb Na}) \\
 &\quad + (473.65 \text{ lb NaH formed})(1053.52 \text{ Btu/lb NaH}) \\
 &= (15,743,778 \text{ Btu in atmosphere and pool})
 \end{aligned}$$

Subroutine EMVBAL would iterate to find the cell temperature at 600°F; that is, the water release would heat the cell from 500°F to 600°F. The components of this cell energy are as follows:

	Mass lb	600°F Unit Energy Btu/lb	Component Energy Btu
Atmosphere energy:			
Hydrogen	0.248	1,480.06	367
Nitrogen	132.76	107.65	14,292
Sodium Vapor	0.0036	2,130	8
Sodium Oxide	619.27	180.65	111,871
Hydrogen in NaH	19.894	1,480.06	29,444
Sodium in NaH	453.75	335.00	152,006
Pool Energy			
Sodium	46,075.8	335.00	<u>15,435,790</u>
Total			15,743,778

The code treats sodium hydride as a special material that does not occupy space in the cell and does not have energy in excess of the energy of its hydrogen and sodium ingredients.

440-lb Carbon Dioxide Release at 1700°F into Air-Filled Cell

The input data cards (for example, Cards 6 and 7 for Cell C) define this cell as having 122,180 ft³ of air (21% oxygen) with 100% relative humidity (for water vapor) and 100°F and 14.7 psia. The initial conditions of this cell are as follows:

p.B.33

Atmosphere mass:

$$M_a = (\underline{349.82 \text{ lb H}_2\text{O}} + \underline{6190.22 \text{ lb N}_2} + \underline{1879.50 \text{ lb O}_2})$$

*Case 13,
p.13*

Atmosphere energy:

$$U_a = (\underline{500,795 \text{ Btu}})$$

The concrete dioxide release transient requires integration of the following portions of the mass and energy differential equations for the cell:

Atmosphere mass:

$$\frac{dM_a}{dt} = \sum_N R_{\text{CO}_2} \quad (3.6.12)$$

Atmosphere energy:

$$\frac{dU_a}{dt} = \sum_N U_{\text{CO}_2} R_{\text{CO}_2} \quad (3.6.13)$$

With the maximum 440-lb carbon dioxide release and associated energy already cited, the final conditions of this cell would be:

Atmosphere mass:

$$M_a = (440.00 \text{ lb CO}_2 + 349.82 \text{ lb H}_2\text{O} + 6190.22 \text{ lb N}_2 + 1,879.50 \text{ lb O}_2)$$

Atmosphere energy:

$$U_a = (663,617 \text{ Btu})$$

Subroutine EMVBAL would iterate to find the cell temperature at 200°F; that is, the carbon dioxide release would heat the cell from 100°F to 200°F.

440-lb Carbon Dioxide Release at 1700°F into Inerted Cell with Sodium Pool

p.B.33 The input data cards (for example, Cards 8 and 9 for Cell D) define this cell as having 1317 ft³ of nitrogen with no oxygen or water vapor at 500°F and 1.47 psia and with a 65,805 lb sodium pool at 500°F. The initial conditions of this cell are as follows:

Atmosphere mass:

*Case 13,
p.13*

$$M_a = \frac{1.5 \times 10^{-4} \text{ lb Na} + 5.26 \text{ lb N}_2}{}$$

Sodium pool mass:

$$M_p = (\underline{65,805 \text{ lb Na}})$$

Atmosphere energy:

$$U_a = (\underline{469 \text{ Btu}})$$

Pool energy:

$$U_p = (\underline{19,988,000 \text{ Btu}})$$

Again, input to the CACECO code must specify the destination of this concrete carbon dioxide release and, in particular with a sodium pool, whether the release enters the atmosphere or the pool of the cell. The chemical reaction of sodium and carbon dioxide is:

but, sodium vapor reacts in the atmosphere and sodium liquid reacts in the pool. In the atmosphere, the heat of this chemical reaction is 3800 Btu/lb Na vapor and in the pool, 1988 Btu/lb Na liquid. In these cases, Card Series 2801 specifies that the carbon dioxide release enters the sodium pool. The concrete carbon dioxide release transient requires integration of the following portions of the mass and energy differential equations for the cell:

Atmosphere mass:

$$dM_a/dt = R_C + R_{\text{Na}_2\text{O}} + B \quad (3.6.15)$$

Sodium pool mass:

$$dM_p/dt = \sum_N R_{\text{CO}_2} - R_{\text{Na}_2} + \text{CO}_2 - B \quad (3.6.16)$$

Atmosphere energy:

$$dU_a/dt = U_g B \quad (3.6.7)$$

Pool Energy:

$$DU_p/dt = \sum_N U_{\text{CO}_2} R_{\text{CO}_2} + Q_{\text{Na}} + \text{CO}_2 - U_g B \quad (3.6.17)$$

The new feature of this case is the chemical reaction between the pool sodium and carbon dioxide release. This reaction,

has the attendant stoichiometric relation of

$$4(22.991 \text{ lb Na/atom}) + (44.010 \text{ lb CO}_2/\text{mole}) \\ = 2 (61.982 \text{ lb Na}_2\text{O/mole}) + (12.010 \text{ lb C/atom})$$

For this case, the stoichiometric relation has 919.43 lb sodium reacting with the maximum 440-lb carbon dioxide release to form 1239.36 lb sodium oxide and 120.07 lb carbon. The energy effects of this carbon dioxide release and chemical reaction in the cell are most easily solved by adding Equations 3.6.7 and 3.6.17 and then integrating:

$$U'_a + U'_p = U_a + U_p + \sum_N U_{\text{CO}_2} R_{\text{CO}_2} + Q_{\text{Na} + \text{CO}_2} \quad (3.6.18) \\ = (469 \text{ Btu in atmosphere}) + (19,988,000 \text{ Btu in pool}) \\ + (162,822 \text{ Btu in carbon dioxide release at } 1700^\circ\text{F}) \\ + (919.43 \text{ lb Na reacted with carbon dioxide})(1988 \text{ Btu/lb Na}) \\ = (21,979,118) \text{ Btu in atmosphere and pool}$$

Subroutine EMVBAL would iterate to find the cell temperature at 600°F ; that is, the carbon dioxide release would heat the cell from 500°F to 600°F .

The components of this cell energy are as follows:

	Mass lb	600°F Unit Energy Btu/lb	Component Energy Btu
Atmosphere energy:			
Nitrogen	5.26	107.65	566
Sodium Vapor	0.00013	2,130	-
Sodium Oxide	1,239.36	180.65	223,890
Carbon	120.07	156.19	18,754
Pool Energy:			
Sodium	64,885.57	335.00	<u>21,735,908</u>
	Total		21,979,118

Debug Cases 13, 14 and 15 were planned to demonstrate the accuracy of code input for specifying the destination of water and carbon dioxide releases from any concrete structure and the attendant material and energy effects in any cell. There were six structures and four cells, and the plan had the releases of a pair of structures directed into an air-filled cell and the release of each structure directed, at least once, into an inerted cell filled with sodium. Further, the contents of the cells were rotated among the cells. This plan is summarized below.

<u>Item</u>	<u>Humid Air</u>	<u>Nitrogen and Pool</u>	<u>Humid Air</u>	<u>Nitrogen and Pool</u>
Expected releases:	H ₂ O of 2 structures	H ₂ O of 1 structure	CO ₂ of 2 structures	CO ₂ of 1 structure
Case 13: Cells	A	B	C	D
Structures	2 and 3	1	5 and 6	4
Case 14: Cells	B	C	D	A
Structures	1 and 3	2	4 and 6	5
Case 15: Cells	C	D	A	B
Structures	1 and 2	3	4 and 5	6

The material and energy results of Cases 13, 14 and 15 are summarized in Table 3.24. In all instances, the water or carbon dioxide released from a structure did appear in the specified cell. Of course, the material released into the sodium pools appeared as the sodium oxide and sodium hydride reaction products. The material balances between the concrete structure releases and specified cells are accurate. Further, the energy balances are accurate. This is most easily checked with the carbon dioxide releases into the air-filled cell, which was sized so that the 162,822 Btu associated with the 440-lb material release would heat the cell 100°F. In Case 13 for example, the 146,152 Btu associated with the 591.6 lb release into Cell C should have heated the cell:

$$(100^{\circ}\text{F})(146,152 \text{ Btu into Cell C})/(162,822 \text{ Btu planned}) = 89.8^{\circ}\text{F}.$$

The CACECO cell heating, shown in Table 3.24, was 86.5°F, the lower rise being due to higher material release. The similar results for this air-filled cell are summarized below.

<u>Case</u>	<u>Cell</u>	<u>Temperature Rise Due to Energy Associated with CO₂ Release</u>	<u>Table 3.24 Rise</u>
13	C	89.8°F	86.5°F
14	D	84.0	82.6
15	A	73.0	72.6

Another check of CACECO results uses the cell responses due to the material released into the sodium pool of the cells. This check assumes that the pool temperature rise is linear with the amount of material released into the cell: the 100°F rise for the 180-lb water release into the 46,989 lb pool and also for the 440-lb carbon dioxide release into the 65,805 pool. This check is similar to that shown in Table 3.23, which itself was due to each release being linear with the temperature rise of the structure and thereby proportional to the change in sensible energy of the structure. The check of cell responses is shown in Table 3.25. The check substantiates the accuracy of the CACECO results for cell responses to material releases. Also, the check shows that the four cells are independent of one another.

TABLE 3.24

RESULTS OF CASES 13, 14 and 15
(Data at $t = 10$ hr unless otherwise noted)

Item	Humid Air	Humid Air	Nitrogen and Sodium Pool	Nitrogen and Sodium Pool	
Maximum structure releases: material associated energy	360 lb H ₂ O 449,824 Btu	880 lb CO ₂ 325,644 Btu	180 lb H ₂ O 224,912 Btu	440 lb CO ₂ 162,822 Btu	
Initial temperature materials	100°F <u>75.4 lb H₂O</u>	100°F <u>0.0 lb CO₂</u>	500°F <u>0.0 lb H₂O</u>	500°F <u>0.0 lb CO₂</u>	Case 13, p.12
Case 13: cells structures	Cell A 2 and 3	Cell C 5 and 6	Cell B 1(slab)	Cell D 4(slab)	
Structure release associated energy	242.6 lb H ₂ O 261,164 Btu	591.6 lb CO ₂ 146,152 Btu	62.8 lb H ₂ O <u>77,336 Btu</u>	153.0 lb CO ₂ <u>54,550 Btu</u>	Case 13, p.27
Cell temperature materials	<u>154.9°F</u> <u>318.0 lb H₂O</u>	<u>186.5°F</u> <u>591.6 lb CO₂</u>	<u>535.0°F</u> <u>216.1 lb Na₂O</u> <u>166.0 lb NaH</u>	<u>534.7°F</u> <u>430.8 lb Na₂O</u>	Case 13, p.29
Case 14: cells structures	Cell B 1 and 3	Cell D 4 and 6	Cell C 2 (cyl.)	Cell A 5 (cyl.)	
Structure releases associated energy	198.8 lb H ₂ O 223,876 Btu	484.5 lb CO ₂ 136,835 Btu	<u>106.6 lb H₂O</u> <u>114,595 Btu</u>	<u>259.8 lb CO₂</u> <u>63,921 Btu</u>	Case 14, p.28
Cell temperature materials	<u>150.1°F</u> <u>274.1 lb H₂O</u>	<u>182.6°F</u> <u>484.5 lb CO₂</u>	<u>558.2°F</u> <u>366.7 lb Na₂O</u> <u>281.7 lb NaH</u>	<u>557.5°F</u> <u>731.8 lb Na₂O</u>	Case 14, p.28
Case 15: cells structures	Cell C 1 and 2	Cell A 4 and 5	Cell D 3(sph.)	Cell B 6(sph.)	
Structure releases associated energy	169.5 lb H ₂ O 192,324 Btu	413.0 lb CO ₂ 118,953 Btu	136.0 lb H ₂ O <u>146,571 Btu</u>	331.8 lb CO ₂ <u>82,245 Btu</u>	Case 15, p.29
Cell temperature materials	<u>145.5°F</u> <u>244.9 lb H₂O</u>	<u>172.6°F</u> <u>413.0 lb CO₂</u>	<u>574.1°F</u> <u>468.0 lb Na₂O</u> <u>359.1 lb NaH</u>	<u>573.4°F</u> <u>934.6 lb Na₂O</u>	Case 15, p.29

TABLE 3.25

CHECK CASES 13, 14 and 15 SODIUM POOL RESPONSES

<u>Item</u>	<u>Temperature Rises, °F</u>		<u>Fraction</u>
	<u>CACECO</u> <u>Results</u>	<u>Planned</u> <u>Value</u>	
Slab Geometry: analytical solution in Figure 11 of Carslaw and Jaeger, Volume integral of temperature			0.359
Case 13, Structure 1 release of H ₂ O into Cell B	35.0	100	0.350
Case 13, Structure 4 release of CO ₂ into Cell D	34.7	100	0.347
-----			-----
Cylindrical Geometry: analytical solution in Figure 24 of Carslaw and Jaeger, Volume integral of temperature			0.613
Case 14, Structure 2 release of H ₂ O into Cell C	58.2	100	0.582
Case 15, Structure 5 release of CO ₂ into Cell A	57.5	100	0.575
-----			-----
Spherical Geometry: analytical solution in Figure 29 of Carslaw and Jaeger, Volume integral of temperature			0.774
Case 15, Structure 3 release of H ₂ O into Cell D	74.1	100	0.741
Case 15, Structure 6 release of CO ₂ into Cell B	73.4	100	0.734

The following additional checks of CACECO code input and results for concrete heat structures were made by these three debug cases. For all, material No. 2 was identified as concrete on Card Series 2201 (input additional heat capacity) and 2301 (input thermal conductivity). This concrete was used in Structures 1 through 6, which were the slab, cylindrical and spherical structures that released water and carbon dioxide.

1. In Case 13, Structures 7 to 12 were similar to Structures 1 to 6 except that Structures 7 to 9 were of material No. 1 and Structures 10 to 12 were of material No. 3. The properties of all materials input in Card Series 300001 for Case 13 were as follows:

<u>Structures</u>	<u>Material No.</u>	<u>Thermal Conductivity Btu/hr-ft-°F</u>	<u>Volumetric Heat Capacity Btu/ft³-°F</u>
7 through 9	1	<u>0.7</u>	<u>59.92</u>
1 through 6	2 "concrete"	<u>0.8</u>	<u>39.0</u>
10 through 12	3	<u>0.5</u>	<u>112.94</u>

p.B. 35

The Case-13 results showed that the temperatures of Structures 7 to 9 were identical to those of Structures 1 to 3, respectively, and the temperatures of Structures 10 to 12 were identical to those of Structures 4 to 6, respectively.

2. In Case 14, Structures 7 to 12 were again similar to structures 1 to 6 except that Structures 7 to 9 were of material No. 1 and Structures 10 to 12 were of material No. 3. The properties of all materials input in Card Series 300001 Case 14 were as follows:

<u>Structures</u>	<u>Material No.</u>	<u>Thermal Conductivity Btu/hr-ft-°F</u>	<u>Volumetric Heat Capacity Btu/ft³-°F</u>
7 through 9	1	<u>0.7</u>	<u>39.0</u>
1 through 6	2 "concrete"	<u>0.8</u>	<u>39.0</u>
10 through 12	3	<u>0.5</u>	<u>39.0</u>

p.B. 38

The Case-14 results showed that the temperatures of Structure 7 to 9 were higher than those of Structure 1 to 3, respectively, and the temperatures of Structures 10 to 12 were higher even more than those of Structures 4 to 6, respectively. The higher temperatures were due to the thermal diffusivities of material No's 1 and 3 being higher than that of material No. 2. Thus, at $t = 10$ hr, Structure 7 to 9 were at Fourier Number $\kappa t/l^2 = 0.154$ and Structures 10 to 12 were at $\kappa t/l^2 = 0.290$, while structures 1 to 6 were only at $\kappa t/l^2 = 0.1$ as shown in Figure 3.20 to 3.22.

3. In Case 15, Structure 7 to 12 were similar to Structure 1. In this case, Card Series 2301 (input thermal conductivity) identified material No's 1 and 2 as having variable thermal conductivity and Card Series 2201 (input additional heat capacity) identified material No's 2 and 3 as being concrete. The properties of all materials input in Card Series 300001 for Case 15 were as follows:

<u>Structures</u>	<u>Material No.</u>	<u>Thermal Conductivity Btu/hr-ft-°F</u>	<u>Volumetric Heat Capacity Btu/ft³-°F</u>
7	1	<u>1.4</u>	<u>59.92</u>
1 to 6, 7, 8, 10, 11 and 12	2 "concrete"	<u>1.4</u>	<u>39.0</u>
8 and 9	3 "concrete"	<u>0.7</u>	<u>39.0</u>
9	4	<u>0.7</u>	<u>59.92</u>

Structures 7, 8 and 9 were composed of alternate regions of materials for the 10 regions of each structure. Structure 7 had material No's 1, 2, 1, 2, etc., and material No. 1 did not release water. Structure 8 had material No's 2, 3, 2, 3, etc., and both materials were concrete. Structure 9 had material No's 3, 4, 3, 4, etc., and material No. 4 did not release water. Structure 10 had 700°F input on Card Series 2601

as the temperature at which water release begins. Structure 11 had an initial temperature of 1200⁰F. Structure 12 was omitted from the input on Card Series 2601. The CACECO results of these structures are compared to the results of Structure 1 at t = 10 hr.

p.B.43

<u>Structure</u>	<u>Comment</u>	<u>Water Release lb</u>	<u>Energy Transferred Btu</u>
1	Slab, material No. 2	<u>62.7</u>	<u>-191,154</u>
7	Mat. No's 1, 2, 1, 2, etc.	<u>27.2</u>	<u>-191,154</u>
8	Mat. No's 2, 3, 2, 3, etc.	<u>62.7</u>	<u>-191,154</u>
9	Mat. No's 3, 4, 3, 4, etc.	<u>35.6</u>	<u>-191,154</u>
10	Release to begin at 700 ⁰ F	<u>0.0</u>	<u>-191,154</u>
11	1200 ⁰ F initial temperature	<u>180.0</u>	<u>+157,280</u>
12	Omitted from Card Series 2601	<u>0.0</u>	<u>-191,154</u>

Case 15,
pp.27,28,29

The water releases of Structures 7 and 9 complement each other and sum to the release of Structures 1 or 8: 62.7 lb. The surface temperature of Structure 10 was always below 700⁰F, and no water was released even though the energy transferred (absorption) was as if water had been released. The initial temperature of Structure 11 caused all of its concrete water to be released as an initial condition. Also, Structure 11 had less energy transferred (note sign) because it cooled and used the cooling-heat capacity of 39 Btu/ft³-⁰F. Finally, Structure 12 had no water released even though the energy transferred was as if water was released. The omission of Structure 12 from Card Series 2601 was done to show the result of this kind of blunder.

4. These three debug cases were used to illustrate the effect that time step has on the results. The Card Series 9001 were used to input different initial step and thereby obtain a different maximum step (10 times the natural step). The effects are illustrated with the results for Structure 1.

	<u>Case</u>	<u>Card Series 9001 Input Step</u>	<u>Water Released lb</u>	<u>Energy Transferred Btu</u>
<i>Case 13, pp. 27 28</i>	13	0.002 hr	<u>62.8</u>	<u>203,860</u>
<i>Case 14, pp. 26, 27</i>	14	0.004	<u>62.8</u>	<u>199,282</u>
<i>Case 15, p. 27</i>	15	0.008	<u>62.7</u>	<u>191,154</u>

These Cases 13, 14, and 15 have shown that CACECO provides accurate analyses of the concrete heat structures, their energy transfers, and the material and energy effects of the water and carbon dioxide releases into the cells. Overall, the check has confirmed the independence of the heat structures and of the cells.

3.7 DEBUG CASES 16 TO 19, FISSION PRODUCT HEATING AND SPACE COOLER OPERATION

Debug Case 16 checks simultaneously the thermal effects of the following four independent situations:

- 1.) In Cell A, fission products heat the 96.7% nitrogen, 3.3% oxygen atmosphere.
- 2.) In Cell B, fission products heat the 6880-lb water pool.
- 3.) In Cell C, fission products and the sodium-oxygen chemical reaction heat the 6880-lb sodium pool.
- 4.) In Cell D, fission products heat the 88.6% nitrogen, 2.0% oxygen, 9.4% water vapor atmosphere, while a space cooler operates to dehumidify and cool the atmosphere.

Debug Cases 17, 18 and 19 check these same situations but in different cells. These four cases have no heat structures and no cell leakage. These cases check the operation of the following input data cards:

Cell data:	Cards 2, 4, 6 and 8 3, 5, 7 and 9
Decay-power history	Card series 101
Factors apportioning Decay power among atmospheres	Card series 201
Factors apportioning decay power among pools	Card series 301
Space-cooler data	Cards 1700, 1800, 1900 and 2000

Each case uses all four cells provided in the code. Each cell has a different volume and initial conditions in order to continue to show the independence of these cells. Cases 16 to 19 rotate these four situations among the four cells.

The same decay-power history was used for these cases. This history was input by Card Series 101 and is listed below; it decreases linearly and (by inspection) averages $Q_{dp} = 160,000$ Btu/hr over the time period from $t = 0$ hr to $t = 1$ hr.

<u>Time t, hr</u>	<u>Decay Power Q_{dp}, Btu/hr</u>	
<u>0.00</u>	<u>210,000</u>	
<u>0.01</u>	<u>209,000</u>	
<u>0.05</u>	<u>205,000</u>	
<u>0.10</u>	<u>200,000</u>	
<u>0.20</u>	<u>190,000</u>	
<u>0.30</u>	<u>180,000</u>	
<u>0.40</u>	<u>170,000</u>	
<u>0.50</u>	<u>160,000</u>	Intended "Average" value
<u>0.60</u>	<u>150,000</u>	
<u>0.70</u>	<u>140,000</u>	
<u>0.80</u>	<u>130,000</u>	
<u>0.90</u>	<u>120,000</u>	
<u>1.00</u>	<u>110,000</u>	

p.B.44

every power history input by Card Series 101 is processed by Subroutine TIMEDP in two steps:

1. The initial time (required to be $t = 0.0$ hr for all histories input to the code) is replaced by the value $t = 1.0 \times 10^{-6}$ hr.
2. The natural logarithm of each time and power value is stored for subsequent use by Subroutine DECPOW.

The CACECO code calls Subroutine DECPOW at the time decay power is required by code calculations, and this subroutine interpolates linearly the logarithmic time and power data to return the decay-power value.

The code uses the decay-power history for two purposes: (1) to provide the time-dependent volumetric heat generation power for the heat structures and (2) to provide the fission-product heating of the atmosphere or pool of any cell. The first purpose, volumetric heat in the heat structures, was discussed in Section 3.3 in connection with Debug Case 9. The second purpose, fission-product heating of cell atmosphere and pool, is discussed here. This fission-product heating depends upon two apportioning factors: F_a for the atmosphere, which is input by Card Series 201; and F_p for the pool, which is input by Card Series 301. These factors transform the decay-power value, Q_{DP} , into the fission-product power, Q_{FP} , in the following portions of the energy differential equations for the cell.

Atmosphere energy:

$$dU_a/dt = Q_{FP} = F_a Q_{DP} \quad (3.7.1)$$

Pool energy:

$$dU_p/dt = Q_{FP} = F_p Q_{DP} \quad (3.7.2)$$

In the integration of these equations, say from $t = t_1$ to $t = t_2$, the code uses the decay-power value at the half-step times, $t_{\frac{1}{2}}$:

$$t_{\frac{1}{2}} = t_1 + (t_2 - t_1)/2 \quad (3.7.3)$$

For example, Case 16 takes steps which are $t_2 - t_1 = 0.1$ hr long. The first step needs the decay-power value at $t_{\frac{1}{2}} = 0.05$ hr, and Subroutine DECPOW finds this time in the table with power $Q_{DP}(0.05 \text{ hr}) = 205,000$ Btu/hr. The second step needs the decay-power value at $t_{\frac{1}{2}} = 0.15$ hr, and Subroutine DECPOW does the interpolation summarized below:

<u>Time hr</u>	<u>Logarithm of Time</u>	<u>Power Btu/hr</u>	<u>Logarithm of Power</u>
0.10	-2.302 58	200,000	12.206 1
0.15	-1.897 12		
0.20	-1.609 44	190,000	12.154 8

$$F_I = \frac{\ln(t_{\frac{1}{2}}) - \ln(t_1)}{\ln(t_2) - \ln(t_1)} = \frac{(-1.897 12) - (-2.302 58)}{(-1.609 44) - (-2.302 58)} = \frac{+0.405 46}{+0.693 15} \\ = (0.584 963)$$

$$\ln(Q_{\frac{1}{2}}) = \ln(Q_1) + F_I [\ln(Q_2) - \ln(Q_1)] \\ = (12.206 1) + (0.584 963) [(12.154 8) - (12.206 1)] \\ = \ln(194,088 \text{ Btu/hr})$$

The value returned by the subroutine, $Q_{DP}(0.15 \text{ hr}) = 194,088$ Btu/hr, is less than the value obtained by linear interpolation of the input data (195,000 Btu/hr) by about 0.47%. In fact, this linear interpolation of the logarithmic history data over the time period, $t = 0$ hr to $t = 1$ hr, made the average power value $Q_{DP} = 159,640$ Btu/hr, which is 0.22% less than the intended value.

3.7.1 Fission Products Heat 96.7% Nitrogen - 3.3% Oxygen Atmosphere

The situation with fission products heating an atmosphere of 96.7% nitrogen and 3.3% oxygen occurs in Cell A of Case 16. The initial conditions of this cell were defined by input data on Card 2 to provide the following atmosphere mass and energy at 200°F:

Atmosphere mass:

$$M_a = (\underline{191.33 \text{ lb N}_2} + \underline{7.46 \text{ lb O}_2})$$

Atmosphere energy:

$$U_a = (\underline{6864.05 \text{ Btu}})$$

This case was planned so that this cell would heat 100°F in 1.0 hr. The apportioning factor for this cell, $F_a = \underline{0.022099}$, provided

$$\begin{aligned} Q_{FP}(t_2 - t_1) &= F_a Q_{FP} (t_2 - t_1) \\ &= (0.22 \ 099)(159,640 \text{ Btu/hr})(1.0 \text{ hr} - 0.0 \text{ hr}) \\ &= (3527.88 \text{ Btu}) \end{aligned}$$

of fission-product heat. The cell conditions at 1.0 hr were as follows:

Atmosphere mass:

$$M_a = (\text{same as at beginning})$$

Atmosphere energy:

$$U_a = (\underline{10,391.94 \text{ Btu}})$$

Subroutine EMVBAL found that the atmosphere was now at 300.00°F.

3.7.2 Fission Products Heat 6,880-lb Water Pool

The situation with fission products heating a water pool in a cell filled with nitrogen, oxygen and water vapor occurs in Cell B of Case 16. The initial conditions of this cell were defined by input data on Cards 5 and 4 to provide the following mass and energy conditions at 100°F:

Atmosphere mass:

$$M_a = (\underline{55.69 \text{ lb } N_2} + \underline{2.93 \text{ lb } O_2} + \underline{0.03 \text{ lb } H_2O})$$

*Case 16,
p.4*

Pool mass:

$$M_p = (\underline{6880.17 \text{ lb } H_2O})$$

Atmosphere energy:

$$U_a = (\underline{1031 \text{ Btu}})$$

Pool energy:

$$U_p = (\underline{470,216 \text{ Btu}})$$

This case was planned so that this water pool would heat 100°F in 1.0 hr.

The apportioning factor for this pool, $F_p = \underline{4.47320}$, provided

p.B.44

$$\begin{aligned} Q_{FP}(t_2 - t_1) &= F_p Q_{DP} (t_2 - t_1) \\ &= (4.473 \text{ } 20)(159,640 \text{ Btu})(1.0 \text{ hr} - 0.0 \text{ hr}) \\ &= (714,102 \text{ Btu}) \end{aligned}$$

of fission-product heat. The cell conditions at 1.0 hr were as follows:

Atmosphere and pool masses:

$$M_a + M_p = (\text{same } N_2 \text{ and } O_2 \text{ as at beginning} + 6880.20 \text{ lb } H_2O)$$

Atmosphere and pool energies:

Case 16,
p.11

$$U_a + U_p = (1,185,350 \text{ Btu})$$

Subroutine EMVBAL found that the cell was now at 200°F, that the atmosphere had 29.54 lb water vapor, and that the pool had 6850.66 lb water liquid.

3.7.3 Fission Products Heat 6,880-lb Sodium Pool

The situation with fission products heating a sodium pool in a cell filled with nitrogen and initial 1.1% oxygen occurs in Cell C of Case 16. The initial conditions of this cell were defined by input data on Cards 7 and 6 to provide the following mass and energy conditions at 400°F:

Atmosphere mass:

Case 16,
p.4

$$M_a = (\underline{600.62 \text{ lb } N_2} + \underline{7.63 \text{ lb } O_2})$$

Pool mass:

$$M_p = (\underline{6880.2 \text{ lb } Na})$$

Atmosphere energy:

Case 16,
p.4

$$U_a = (\underline{42,865 \text{ Btu}})$$

Pool energy:

$$U_p = (\underline{1,871,800 \text{ Btu}})$$

This cell included the sodium-oxygen reaction which was discussed in Section 3.1.2. The 7.63 lb oxygen reacted with 21.93 lb sodium vapor to produce 29.56 lb sodium oxide and 125,983 Btu of chemical reaction energy. This chemical reaction heated the pool 55.8°F in one time step. This case was planned so that the sodium pool would heat 100°F in 1.0 hr. The apportioning factor for this pool, $F_p = 0.63485$, provided $Q_{FP} (t_2 - t_1) = 101,348$ Btu of fission-product heat. The cell conditions at 1.0 hr were as follows:

p.B.44

Atmosphere and pool masses:

$$M_a + M_p = (\underline{600.62 \text{ lb } N_2} + \underline{6858.27 \text{ lb } Na} + \underline{29.56 \text{ lb } Na_2O})$$

*Case 16,
p.11*

Atmosphere and pool energies:

$$U_a + U_p = (\underline{2,140,996 \text{ Btu}})$$

Subroutine EMVBAL found that the cell was now at 500°F.

3.7.4 Fission-Product Heating Controlled by Space Cooler

The situation with fission products heating an atmosphere of 92.0% nitrogen, 2.1% oxygen and 5.9% water vapor occurs in Cell D of Case 16. The initial conditions of this cell were defined by input data on Cards 9 and 8 to provide the following atmosphere mass and energy at 300°F:

Atmosphere mass:

$$M_a = (\underline{15.54 \text{ lb } H_2O} + \underline{378.07 \text{ lb } N_2} + \underline{9.71 \text{ lb } O_2})$$

*Case 16,
p.4*

Atmosphere energy:

$$U_a = (\underline{37,450 \text{ Btu}})$$

*Case 16,
p.4*

This case was planned in three steps. The first plan had the dry atmosphere of nitrogen and oxygen heated from 300°F to 400°F in 1.0 hr and used the apportioning factor of $F_a = 0.045035$ to provide 7189 Btu of fission-product heat. The second plan modified the first by activating a space cooler from 0.20 to 0.60 hr, which was sized to remove the fission-product heat so that the atmosphere returned to 300°F at 1.0 hr. The third plan modified the second by adding 15.54 lb water vapor to the initial atmosphere and increasing the space-cooler size in order to demonstrate that the space cooler will dehumidify the atmosphere before cooling it.

The space cooler calculations were covered in Section 3.1.3. In the present case, the cooler was assumed to operate according to the equation

p.B.44

$$Q_{SC} = 57,540.0 + 80.0 (T_a - 200.0^\circ\text{F})$$

for $0.2 \text{ hr} \leq t \leq 0.60 \text{ hr}$ so long as $T_a > 250^\circ\text{F}$ where Q_{SC} (Btu/hr) is the space-cooler duty at t (hr) time and T_a (°F) atmosphere temperature. The space-cooler calculations are done in Subroutine COOLR. These calculations include the duty calculations described in Section 3.1.3 and a check for water vapor in the cell atmosphere. The subroutine assumes that the space cooler will dehumidify the atmosphere before cooling it. The code solves the following equations:

Atmosphere energy:

$$dU_a/dt = Q_{FP} - Q_{SC} \quad (3.7.4)$$

Atmosphere mass of water vapor:

$$dM_a/dt = -Q_{SC}/U_g \quad (3.7.5)$$

In the above equations U_g (Btu/lb water) is the energy of water vapor at temperature T_a .

These equations were used to calculate the following steps for Cell D of Case 16:

Time hr t	Atm. Temp. °F T_a	Atm. Energy Btu U_a	Decay Power Btu/hr Q_{FP}	Cooler Duty Btu/hr Q_{SC}	Energy Change Btu/hr dU_a/dt	Water Energy Btu/hr U_g	Water Mass Change lb/hr dM_a/dt	Atm. Water Mass lb M_a
0.20	<u>324.0</u>	<u>39,249</u>	- 8,306	- <u>67,457</u>	- 59,151	1112.3	- 60.6	<u>15.54</u>
0.30	<u>335.3</u>	<u>33,334</u>	- 7,861	- <u>68,365</u>	- 60,503	1116.2	- 61.2	<u>9.48</u>
0.40	<u>346.4</u>	<u>27,283</u>	- 7,415	- 37,562	- 30,147	1120.1	- 33.5	<u>3.35</u>
0.50	<u>356.9</u>	<u>24,268</u>	-	-	-	--	-	<u>0.00</u>

Case 16,
p.6

Case 16,
p.7

Case 16,
p.7

Case 16,
p.8

These calculations were straightforward until the step from 0.40 hr to 0.50 hr, when the calculated cooler duty, $Q_{SC} = \underline{69,249 \text{ Btu/hr}}$, was capable of condensing 6.18 lb of water. However, the atmosphere had only 3.35 lb of water, and the code took this time step as if the cooler duty was only $Q_{SC} = (3.35 \text{ lb})(1120.1 \text{ Btu/lb})/(0.1 \text{ hr}) = 37,562 \text{ Btu/hr}$, as listed above. In a sense, the space cooler stopped its dehumidification at 0.45 hr and should have begun cooling immediately thereafter.

Case 16,
p.8

The Cell D conditions at 1.0 hr were as follows:

Atmosphere mass:

$$M_a = (\underline{378.07 \text{ lb}} \text{ N}_2 + \underline{9.71 \text{ lb}} \text{ O}_2)$$

Case 16,
p.12

Atmosphere energy:

$$U_a = (\underline{20,295 \text{ Btu}})$$

Subroutine EMVBAL found that the cell was now back to 300°F.

3.7.5 Cell Independence

Debug Cases 17, 18 and 19 check the same situations as Case 16, but in different cells. These four situations and their summary results for Cases 16 through 19 are summarized in Table 3.26. These results show that in these situations the four cells are independent of on another.

These four debug cases were used to illustrate the effect that time step has on the results. With these no-leakage situations, the only one which was dependent upon the time step was that with the space cooler because the cooler was to have started at 0.20 hr, finished dehumidification at 0.45 hr and stopped at 0.80 hr. These start, dehumidification and stop times were not matched exactly; thus, there is variation in the final temperature of the cell illustrating this situation.

TABLE 3.26

DEBUG CASES 16 THROUGH 19

<u>Situation</u>	<u>Fission Products Heat Atmosphere</u>		<u>Fission Products Heat Water Pool</u>		<u>Fission Products and Chemical Reaction Heat Sodium Pool</u>		<u>Fission Products Heat and Space Cooler Cools Atmosphere</u>	
Case 16	Cell A		Cell B		Cell C		Cell D	
Case 17	Cell D		Cell A		Cell B		Cell C	
Case 18	Cell C		Cell D		Cell A		Cell B	
Case 19	Cell B		Cell C		Cell D		Cell A	
Cell Volume, ft ³	<u>2,222</u>		<u>1,111</u>		<u>4,444</u>		<u>3,333</u>	
	<u>Time</u>	<u>Time</u>	<u>Time</u>	<u>Time</u>	<u>Time</u>	<u>Time</u>	<u>Time</u>	<u>Time</u>
	<u>0.0 hr</u>	<u>1.0 hr</u>	<u>0.0 hr</u>	<u>1.0 hr</u>	<u>0.0 hr</u>	<u>1.0 hr</u>	<u>0.0 hr</u>	<u>1.0 hr</u>
Pressure, psia	<u>22.5</u>	<u>25.9</u>	<u>11.2</u>	<u>26.3</u>	<u>45.0</u>	<u>51.1</u>	<u>34.8</u>	<u>33.8</u>
Temperature, °F	<u>200.0</u>	<u>300.0</u>	<u>100.0</u>	<u>200.0</u>	<u>400.0</u>	<u>500.0</u>	<u>300.0</u>	<u>300.0</u>
Nitrogen, lb	<u>191.3</u>	<u>191.3</u>	<u>55.7</u>	<u>55.7</u>	<u>600.6</u>	<u>600.6</u>	<u>378.1</u>	<u>378.1</u>
Oxygen, lb	<u>7.4</u>	<u>7.4</u>	<u>2.9</u>	<u>2.9</u>	<u>7.6</u>	<u>0.0</u>	<u>9.7</u>	<u>9.7</u>
Sodium, lb	0.0	0.0	0.0	0.0	<u>6,880.2</u>	<u>6,858.3</u>	0.0	0.0
Sodium oxide, lb	0.0	0.0	0.0	0.0	<u>0.0</u>	<u>29.6</u>	0.0	0.0
Water, lb	0.0	0.0	<u>6,880.2</u>	<u>6,880.2</u>	0.0	0.0	15.5	0.0
<i>Output for Cell A</i>	<i>Case 16</i>	<i>Case 16</i>	<i>Case 17</i>	<i>Case 17</i>	<i>Case 18</i>	<i>Case 18</i>	<i>Case 19</i>	<i>Case 19</i>
	<i>p. 4</i>	<i>p. 11</i>	<i>p. 4</i>	<i>p. 12</i>	<i>p. 4</i>	<i>p. 12</i>	<i>p. 4</i>	<i>p. 12</i>

3.8 DEBUG CASES 20 TO 31, LEAKAGE CALCULATIONS CELL-TO-CELL

Debug Cases 20 to 31 check the leakage calculations of the code. In particular, Case 20 checks simultaneously the following two independent leakage situations:

1. Leak carbon dioxide, nitrogen, oxygen and water vapor from Cell A to Cell B. Maintain the leak rate from Cell A to Cell B constant by holding constant the pressure and density of Cell A and the pressure of Cell B.
2. Leak hydrogen, nitrogen and sodium vapor from Cell C to Cell D. Maintain the leak rate from Cell C to Cell D constant by holding constant the pressure and density of Cell C and the pressure of Cell D.

Debug Cases 20 through 31 check these same leakage situations but for different cell pairs. The objective of these twelve cases was to check all possible cell pair combinations for all gases and vapors. For example, Case 20 checked CO_2 , N_2 , O_2 and H_2O leakage from Cell A to Cell B (forward); Case 23 checked this leakage from Cell B to Cell A (reverse); Case 28 checked H_2 , N_2 and Na leakage from Cell A to Cell B (forward); and, Case 31 checked this leakage from Cell B to Cell A (reverse), thereby checking this cell pair combination for all gases and vapors. The plan of these twelve cases is summarized in Table 3.27.

TABLE 3.27

PLAN OF DEBUG CASES 20 to 31
(The case numbers are listed)

<u>High Pressure Cells at 44.7 psia</u>	<u>CO₂, N₂, O₂ and H₂O Leakage Low Pressure Cells at 34.7 psia</u>			
	<u>Cell A</u>	<u>Cell B</u>	<u>Cell C</u>	<u>Cell D</u>
Cell A	--	20	21	22
Cell B	23	--	24	25
Cell C	26	27	--	28
Cell D	29	30	31	--

<u>High Pressure Cells at 39.7 psia</u>	<u>H₂, N₂ and Na Leakage Low Pressure Cells at 14.7 psia</u>			
	<u>Cell A</u>	<u>Cell B</u>	<u>Cell C</u>	<u>Cell D</u>
Cell A	--	28	25	24
Cell B	31	--	22	21
Cell C	30	29	--	20
Cell D	27	26	23	--

Cases 20 through 31 use the input data cards which describe cell data, air injection, space coolers and concrete heat structures, all of which have been checked before. The present cases concentrate on checking the input data cards which are used to describe cell-to-cell leakage. These are listed below:

High Pressure Cells	Leak Means	Listed are Card and Card Series Numbers Low Pressure Cells			
		Cell A	Cell B	Cell C	Cell D
Cell A	Nozzle	--	10	20	30
	Coefficient	--	11	21	31
Cell B	Nozzle	10	--	50	60
	Coefficient	11	--	51	61
Cell C	Nozzle	20	50	--	80
	Coefficient	21	51	--	81
Cell D	Nozzle	30	60	80	--
	Coefficient	31	61	81	--

3.8.1 Leakage Calculations

The CACECO code has two sets of equations to describe leakage: one set implies a mechanistic leak path through a nozzle; the other set is non-mechanistic and uses a leakage coefficient. Either set of equations can be used, with the choice depending upon the convenience of the code user.

These two sets of equations are summarized below:

- 1.) Nozzle equations are used when the flow area, A (ft^2), and flow coefficient, C , are input on Cards 10, 20, 30, etc. These nozzle equations are for the one-dimensional flow of an ideal compressible gas. They were obtained from the CONTEMPT code description by Richardson, et al.⁽⁹⁾ They are specialized in the CACECO code because the atmosphere being leaked is assumed to have a specific heat ratio of $k = C_p/C_v = 1.361$ as if it were always nitrogen at about 1000°F . This specialization is evident in the below-listed working

equations for leakage from a cell with pressure P_I (psia) and density ρ_I (lb/ft³) to a cell with pressure P_J (psia). The code calculates a pressure ratio,

$$R = P_J/P_I \quad (3.8.1)$$

and a modified pressure ratio,

$$Z = R^{1/k} = R^{0.73475} \quad (3.8.2)$$

The flow is subsonic when the pressure ratio is

$$R > \left(\frac{2}{k+1} \right)^{k^2/(k-1)} > 0.4268 \quad (3.8.3)$$

The subsonic leak rate is then

$$\begin{aligned} L_{IJ} &= A C \sqrt{\frac{2}{k-1} \frac{g}{k} P_I \rho_I Z(Z-R)} \\ &= 672,863 A C \sqrt{P_I \rho_I Z(Z-R)} \end{aligned} \quad (3.8.4)$$

The leakage flow is at sonic velocity through the nozzle when the pressure ratio is $R \leq 0.4268$, and this limiting value (0.42680) is used to calculate the leak rate in Equation 3.8.4.

These nozzle equations were used to size the nozzle area and nozzle coefficient for the two leakage situations of Debug Case 20.

- a. For the leakage from Cell A to Cell B, Cell A was held at pressure $P_A = \underline{44.7 \text{ psia}}$ and density $\rho_A = \underline{0.177525 \text{ lb/ft}^3}$, and Cell B was held at pressure $P_B = \underline{34.7 \text{ psia}}$. The pressure ratio, calculated by Equation 3.8.1 as

*Case 20,
p.7*

$$R = (34.7 \text{ psia})/(44.7 \text{ psia}) = (0.776286)$$

indicated that the flow would be subsonic. The modified pressure ratio was calculated by Equation 3.8.2 as $Z = (0.83022)$. The planning of this debug leakage situation required a leak rate of $L_{AB} = 688.99$ lb/hr, and the evaluation of Equation 3.8.4 gave the product $AC = 0.0017178$ ft². The code processes the individual input values of area, A, and coefficient, C, to make the product, AC, and this permits the code user to input the product in any convenient form. For example, the following are equivalent input on Card 10:

$$(1) \quad A = 0.0017178 \text{ ft}^2 \text{ and } C = 1.000$$

$$(2) \quad A = 0.0021472 \text{ ft}^2 \text{ and } C = 0.800$$

- b. For the leakage from Cell C to Cell D, Cell C was held at pressure $P_C = \underline{39.7 \text{ psia}}$ and density $\rho_C = \underline{0.045917 \text{ lb/ft}^3}$, and Cell D was held at pressure $P_D = \underline{14.7 \text{ psia}}$. The pressure ratio, calculated by Equation 3.8.1 as $R = 0.37028$ indicated that the flow would be sonic and that the value $R = 0.42680$ should be used in Equations 3.8.2 and 3.8.4. The result was the product $AC = 0.00059037$ ft², which could be input on Card 80 as $A = 0.00073796$ ft² and $C = 0.800$.

- 2.) The coefficient equation is used when values of leakage coefficient as a function of differential pressure are input on Card Series 11, 21, 31, etc. This equation is most convenient for the calculation of leakage from a reactor containment building, which may be specified as being 0.1%/day. This specification has been used to mean a leak rate of 0.1% of the building volume in 24 hours when the building is at the design pressure and nominal testing temperature (80°F, for example). the coefficient equation for leak rate is as follows:

$$L_{IJ} = C \sqrt{(P_I - P_J) \rho_I} \quad (3.8.5)$$

This coefficient equation was used to calculate the leakage coefficient for the two leakage situations of Debug Case 20.

- a.) For the leakage from cell A to Cell B with Cell A held at pressure $P_A = 44.7 \text{ psia}$ and density $\rho_A = 0.177525 \text{ lb/ft}^3$ and Cell B held at pressure $P_B = 34.7 \text{ psia}$, the planned leak rate was 688.99 lb/ft^3 and the leakage coefficient from equation 3.8.5 was

Case 20,
p.7

$$C = 517.110 \text{ lb hr} - \sqrt{\text{psia-lb/ft}^3}.$$

- b.) For the leakage from Cell C to Cell D with Cell C held at pressure $P_C = 39.7 \text{ psia}$ and density $\rho_C = 0.045917 \text{ lb/ft}^3$ and Cell D held at pressure $P_D = 14.7 \text{ psia}$, the planned leak rate was 132.438 lb/hr and the leakage coefficient from Equation 3.8.5 was

Case 20,
p.8

$$C = 123.611 \text{ lb/hr} - \sqrt{\text{psia-lb.ft}^3}.$$

The plan of this case used the chemical-engineering methodology of the continuously stirred tank reactor to provide an analytical test of the CACECO leakage calculations. Following this methodology, the higher-pressure cell was treated as a tank reactor with constant mass M and variable composition C_i for component i , which had a feed stream of constant flowrate L and composition C_{i1} and a product stream of constant flowrate L and composition C_{i2} . The assumption of continuously stirred tank was equivalent to the assumption of the well-mixed atmosphere of each cell and made the composition of the product stream the same as the composition of the tank: $C_{i2} = C_i$. The material balance for this component i was then

$$M \, dC_i/dt = L (C_{i1} - C_{i2}) \quad (3.8.6)$$

If the composition of the tank was $C_i = C_{i0}$ at $t = 0$, then the composition at a later time was

$$C_i = C_{i1} + (C_{i0} - C_{i1}) \text{Exp}(-Lt/M) \quad (3.8.7)$$

Each leak situation was planned so that at $t = 1$ hr, the composition of one component was

$$C_i/C_{i1} = 1/2 = \text{Exp}(-Lt/M) = \text{Exp}(-0.693147)$$

or: $L = 0.693147 M$.

3.8.2 Leakage of CO_2 , N_2 , O_2 and H_2O

The leakage situation for carbon dioxide, nitrogen, oxygen and water vapor occurs between Cell A and Cell B of Debug Case 20. The plan for this case noted that:

- 1.) The feed stream of carbon dioxide could come only from heating a limestone-concrete heat structure.
- 2.) The feed stream of nitrogen and oxygen could be set by the air injection described on Card Series 1201, and
- 3.) The feed stream of water vapor could come only from heating another concrete heat structure.

In Cell A, the differential equation for the material balance of the stirred-tank reactor was replaced by the following portion of the differential equation for component i of the cell atmosphere mass:

$$d(M_a)_i/dt = (I_{\text{N}_2 + \text{O}_2})_i + \sum_N (R_{\text{CO}_2})_i + \sum_N (R_{\text{H}_2\text{O}})_i - \sum_K (L_{\text{JK}})_i \quad (3.8.8)$$

Of course, Equations 3.8.6 and 3.8.8 are the same except that Equation 3.8.6 is in terms of the concentration, C_i , and Equation 3.8.8 is in terms of the mass, $(M_a)_i$; that is, $MC_i = (M_a)_i$. The leakage situation was planned so as to comply with the assumptions of Equation 3.8.6. This planning is summarized below in terms of Cell A as the higher-pressure cell and Cell B as the lower-pressure cell.

- 1.) Cell A has the flowing concentration transients which are described in the nomenclature of Equation 3.8.7.

Component <u>i</u>	Feed <u>C_{i1}</u>	Initial <u>C_{i0}</u>	Halfway <u>C_i (0.5 hr)</u>	End of Run <u>C_i (1.0 hr)</u>
CO ₂	0.088	0.000	0.026	0.044
N ₂	0.704	0.704	0.704	0.704
O ₂	0.157	0.245	0.220	0.201
H ₂ O	0.050	0.050	0.050	0.050

- 2.) The constant mass in cell A of $M_a = 994$ lb was obtained by having equal feed and leakage flow rates. These flow rates were each $L = 0.693147 M = \underline{688.99 \text{ lb/hr}}$. The constant mass in Cell A made its density constant also.

Case 20,
p.9

- 3.) The constant feed rate to Cell A had two parts:

- a.) The CO₂ and H₂O feeds were obtained by heating separate concrete heat structures. The materials used in these heat structures were described in Section 3.6 and used previously in Debug Case 13. These properties are linear with temperature: the CO₂ is released at the heating rate of 22.0 lb/ft³-500°F, and the H₂O is released at the rate of 9.0 lb/ft³-500°F. With a steady temperature rise of 100°F/hr in each structure (accomplished by volumetric heating of the structure), the 61.00 lb/hr CO₂ feed was obtained by heating 13.8636 ft³ of concrete above 1200°F, and the 34.66 lb/hr H₂O was obtained by heating 19.2556 ft³ of concrete above 200°F.

p.B.50

p.B.49

b.) The N_2 and O_2 feeds were obtained by input data definition on the Card Series 1201.

4.) The constant leak rate from Cell A to Cell B depended upon constant pressures in each cell. With the objective of maintaining constant pressure P in each cell of volume V , the change in moles of gas and vapor N had to be compensated for by an inverse change in temperature T according to the Ideal Gas Law, $PV = NRT$. The changes in temperature were schedule as follows:

a.) In Cell A, the plan had CO_2 replacing O_2 , and the gradual decrease in mole inventory was compensated by temperature rise from $200^{\circ}F$ to 0 hr to $204.12^{\circ}F$ at 0.5 hr and to $207.07^{\circ}F$ at 1.0 hr. These temperatures were controlled by the energy balance between the feed and leak flows. The plan scheduled the air-injection temperatures to be $152.90^{\circ}F$ from 0 to 0.5 hr, and $143.99^{\circ}F$ from 0.5 to 1.0 hr in order to obtain the Cell-A temperatures desired.

b.) In Cell B, severe cooling from $537^{\circ}F$ at 0 hr to $100^{\circ}F$ at 1.0 hr was required to compensate for the 55.6 lb moles of gas and vapor added to the cell atmosphere by inleakage from Cell A. However, as noted in Section 3.7.4, the space cooler condenses water vapor before cooling the atmosphere, and the continual inleakage with 3.4% water vapor blocked the cooling mode of the cooler. The plan was altered to add 150 lb of sodium oxide as an initial condition of Cell B to dehydrate the gas-vapor inleakage and permit the space cooler to operate in its cooling mode. The cooling duty of this cooler included the enthalpy of the inleakage flow, the chemical reaction energy of the $Na_2O + H_2O \rightarrow 2 NaOH$ reaction, and the $PV = NRT$ compensation for the inleakage of 53.7 lb moles of CO_2 , N_2 and O_2 .

The conditions for this check of CO_2 , N_2 , O_2 and H_2O leakage are summarized in Table 3.28.

TABLE 3.28
CONDITIONS FOR CO₂, N₂, O₂ AND H₂O LEAKAGE CHECK

<u>Items for Cell at 44.7 psia</u>	<u>t = 0 hr</u>	<u>t = 0.5 hr</u>	<u>t = 1.0 hr</u>
Mass composition, CO ₂ , lb	0.000	<u>25.775</u>	<u>44.000</u>
N ₂ , lb	<u>700.000</u>	<u>700.000</u>	<u>700.000</u>
O ₂ , lb	<u>244.000</u>	<u>218.225</u>	<u>200.000</u>
H ₂ O, lb	<u>50.000</u>	<u>50.000</u>	<u>50.000</u>
Total mass of cell, lb	994.000	994.000	994.000
Total lb moles in cell	35.3860	35.1662	35.0108
Temperature, °F	<u>200.00</u>	<u>204.12</u>	<u>207.07</u>
Total energy of cell, Btu	<u>85,588.2</u>	<u>86,358.8</u>	<u>86,911.9</u>
Enthalpy of leakage, Btu/lb	132.727	133.497	134.050
H ₂ O release into cell,			
temperature, °F	<u>200.0</u>	<u>250.0</u>	<u>300.0</u>
energy, Btu/lb	<u>1,072.06</u>	<u>1,087.34</u>	<u>1,103.99</u>
CO ₂ release into cell,			
temperature, °F	<u>1,200.0</u>	<u>1,250.0</u>	<u>1,300.0</u>
energy, Btu/lb	<u>243.75</u>	<u>255.89</u>	<u>268.15</u>
<u>Items for Cell at 34.7 psia</u>	<u>t = 0 hr</u>	<u>t = 0.5 hr</u>	<u>t = 1.0 hr</u>
Mass composition, CO ₂ , lb	0.000	<u>4.725</u>	<u>17.000</u>
N ₂ , lb	<u>0.000</u>	<u>242.600</u>	<u>485.200</u>
O ₂ , lb	<u>1,000.000</u>	<u>1,079.840</u>	<u>1,152.130</u>
H ₂ O, lb	0.000	0.000	0.000
Na ₂ O, lb	<u>150.000</u>	<u>90.378</u>	<u>30.756</u>
NaOH, lb	0.000	<u>76.952</u>	<u>153.900</u>
Total lb moles in cell			
atmosphere	31.2500	42.5117	53.7090
Temperature, °F	502.23	<u>247.41</u>	<u>100.00</u>
Total energy of cell, Btu	104,812.0	<u>64,004.3</u>	<u>24,776.0</u>
<i>Output for Cells A and B</i>	<i>Case 20</i>	<i>Case 20</i>	<i>Case 20</i>
	<i>p. 7 & 15</i>	<i>p. 27</i>	<i>p. 38</i>

Note that this case uses the CACECO code capability for restart to obtain the particular initial conditions desired in Cell B: 150 lb Na₂O and 1000 lb O₂ at 502.23°F and 34.7 psia. In the first start, Cards 4 and 5 define cell conditions to include 10,038.7 lb O₂ and 111.28 lb Na at 80°F. In the first time step to 0.001 hr, the sodium-oxygen reaction makes the 150.0 lb Na₂O desired and raises the cell to 453°F. In the restart, Card 4 redefines the cell conditions to obtain 1000 lb O₂ at 502.23°F and 34.7 psia. The actual temperature input on Card 4, 629.73°F, is that which is necessary to compensate for the (implied) 0°F temperature of the Na₂O in Subroutine INISHL at this restart.

Case 20,
p.7

p.B.49

Case 20,
p.10

p.B.50

3.8.3 Leakage of H₂, N₂ and Na

The leakage situation for hydrogen, nitrogen and sodium vapor occurs between Cell C and Cell D of Debug Case 20. The plan for this case noted that

- 1.) The feed stream of hydrogen could come only from the sodium-water reaction, which implied providing a feed stream of water vapor into a cell with sodium. In turn, the feed stream of water vapor could come only from heating another concrete heat structure.
- 2.) The concentration of sodium vapor in equilibrium with a sodium pool is controlled by the temperature of the pool.

An original plan used the sodium-water reaction to heat a sodium pool and thereby increase the concentrations of both hydrogen and sodium vapor in the cell atmosphere. However, this plan had to be discarded because the cell pressure could not be maintained constant. The sodium pool was convenient because its mass tempered the effects of the chemical reactions. The final plan cooled the cell as hydrogen accumulated. This planning is summarized below in terms of Cell C as the higher-pressure cell and Cell D as the lower-pressure cell.

- 1.) Cell C has the following concentration transients which are describe in the nomenclature of Equation 3.8.7.

Component <u>i</u>	Feed <u>C_{i1}</u>	Initial <u>C_{i0}</u>	Halfway <u>C_i (0.5 hr)</u>	End of Run <u>C_i (1.0 hr)</u>
H ₂	0.014	0.000	0.004	0.007
N ₂	0.960	0.472	0.615	0.716
Na	0.026	0.528	0.381	0.277

- 2.) The nearly constant mass in the atmosphere of Cell C of $M_a = 191.1$ lb was obtained by having equal feed and leakage flow rates. These flow rates were each $L = 0.693147 M = \underline{132.438}$ lb/hr. The constant mass in the Cell C atmosphere made its density constant also.

Case 20,
p.9

- 3.) The constant feed rate to Cell C had three parts:

- a.) The constant H₂O feed to the sodium pool for the generation of H₂ was obtained by heating another concrete heat structure. With correction for the consumption of H₂ by the sodium hydride reaction, the required 16.716 lb/hr of H₂O feed was obtained by volumetric heating 9.2867 ft³ of concrete above 200°F.

p.B.50

- b.) The N₂ feed was obtained by input data on Card Series 1401.

- c.) The Na feed was obtained by evaporating from the sodium pool. The planning covered the sodium balance and noted its consumption by reaction with water and also with hydrogen in addition to its loss by leakage. The plan provided 246.53 lb of pool sodium at the start so as to end with 200.00 lb at 1.0 hr.

p.B.49

- 4.) The constant leak rate from Cell C to Cell D depended upon constant pressures in each cell. Again, the change in moles of gas and vapor in each cell had to be compensated for by an inverse change in temperature according to the Ideal Gas Law. The changes in temperature were planned as follows:

- a.) Cell C temperatures were scheduled to be 1700.0°F at the start, 1623°F at 0.5 hr and 1560.0°F at 1.0 hr. These temperatures were obtained by operating the space cooler in Cell C as defined by Input Card 1900. The cooler duty included the atmosphere and pool cooling, the energy of the water released into the cell from the heat structure, and the energies of the sodium reactions with water and hydrogen. The temperature of the nitrogen injection was set low, at 100.0°F in order to reduce the cooler duty.
- b.) Cell D temperatures were scheduled to cool from 300.0°F at the start to 100.0°F at 1.0 hr. The cooler duty, defined on Input Card 2000, included the atmosphere and pool cooling, the enthalpy of the inleakage of H₂, N₂ and Na, the condensation and freezing of the sodium, and the energy of the sodium reaction with hydrogen.

The conditions for this check of H₂, N₂ and Na leakage are summarized in Table 3.29.

3.8.4 Cell Independence

Debug Cases 21 through 31 check the same leakage situations as Case 20 but for different cell combinations. As noted before, the plan was to check all of the cell combinations for all gases and vapors.

The leak rate calculated by one set of equations is added to the leak rate calculated by the other set when both are operative. That is, the leak rate calculated by the nozzle equation, Equation 3.8.4, is added by the code to the leak rate calculated by the coefficient equation, equation 3.8.5. This addition property of leak rates was checked by varying the proportions of leakage by the two methods. The plan of this check is summarized in Table 3.30. The proportion varied from having all of the leakage by nozzle to having none.

TABLE 3.29
CONDITIONS FOR H₂, N₂ AND Na LEAKAGE CHECK

<u>Items for Cell at 39.7 psia</u>	<u>t = 0 hr</u>	<u>t = 0.5 hr</u>	<u>t = 1.0 hr</u>
Mass composition, H ₂ , lb	0.000	<u>0.783</u>	<u>1.337</u>
N ₂ , lb	<u>90.184</u>	<u>117.494</u>	<u>136.805</u>
Na (vapor), lb	<u>100.884</u>	<u>72.791</u>	<u>52.926</u>
Na (liquid), lb	<u>246.533</u>	<u>222.885</u>	<u>200.000</u>
NaH, lb	0.000	<u>0.269</u>	<u>0.286</u>
Na ₂ O, lb	0.000	<u>29.208</u>	<u>57.708</u>
Total mass of cell atmosphere, lb	191.068	191.068	191.068
Total lb moles in cell atmosphere	7.607	7.748	7.848
Temperature, °F	<u>1,700.0</u>	<u>1,623.9</u>	<u>1,560.0</u>
Total energy of cell, Btu	<u>411,570</u>	<u>357,212</u>	<u>316,570</u>
Enthalpy of leakage, Btu/lb	1,451.7	1,189.6	997.9
H ₂ O release into cell,			
temperature, °F	200.0	<u>250.0</u>	<u>300.0</u>
energy, Btu/lb	1,072.06	<u>1,087.34</u>	<u>1,103.99</u>
 <u>Items for Cell at 14.7 psia</u>	 <u>t = 0 hr</u>	 <u>t = 0.5 hr</u>	 <u>t = 1.0 hr</u>
Mass composition, H ₂ , lb	0.000	<u>0.000</u>	<u>0.000</u>
N ₂ , lb	<u>226.788</u>	<u>263.048</u>	<u>307.308</u>
Na (liquid), lb	0.000	<u>26.530</u>	<u>39.609</u>
NaH, lb	0.000	<u>3.428</u>	<u>12.309</u>
Total lb moles in cell atmosphere	8.095	9.389	10.969
Temperature, °F	<u>300.00</u>	<u>200.00</u>	<u>100.00</u>
Total energy of cell, Btu	<u>11,890</u>	<u>13,900</u>	<u>11, 810</u>
 <i>Output for Cells C and D</i>	 <i>Case 20</i>	 <i>Case 20</i>	 <i>Case 20</i>
	<i>p. 7</i>	<i>p. 27</i>	<i>p. 38</i>

TABLE 3.30
DEBUG CASES 20 THROUGH 31

<u>Item</u>	<u>CO₂ + N₂ + O₂ + H₂O Leakage</u>	<u>H₂ + N₂ + Na Leakage</u>
Cell-to-cell leak rate lb/hr	688.99	132.438
Nozzle leakage, AC product ft ²	0.0017178	0.00059037
Coefficient leakage, coefficient lb/hr $\sqrt{\text{psia-lb/ft}^3}$	517.110	123.611

(Listed below are the leak rates by both methods)

<u>Case</u>	<u>Nozzle</u>	<u>Coefficient</u>	<u>Nozzle</u>	<u>Coefficient</u>
20	0%	100%	100%	0%
21	20	80	80	20
22	40	60	60	40
23	60	40	40	60
24	80	20	20	80
25	100	0	0	100
26	100	0	0	100
27	80	20	20	80
28	60	40	40	60
29	40	60	60	40
30	20	80	80	20
31	0	100	100	0

The results of these debug cases show that the cells are independent of one another and that the cell-to-cell leakage can be operated by either or both the nozzle and coefficient equations as convenient.

3.9 DEBUG CASES 32, 33 AND 34, LEAKAGE CALCULATIONS TO CHECK ENERGY FUNCTIONS AND LEAKAGE CELL-TO-OUTSIDE

Debug Cases 32, 33 and 34 continue the check of the leakage calculations of the code. The leakage situations of these three cases differ from those described in Section 3.8 (Cases 20 to 31) because the cell conditions change during the transients and leakage continues until the cell pressures are equalized. Further, these three cases check the cell-to-outside leakage calculation. The plan of these three cases is summarized in Table 3.31.

TABLE 3.31
PLAN OF DEBUG CASES 32, 33 AND 34

<u>Case</u>	<u>Cell-to-Cell Leakage to Pressure Equalization</u>	<u>Cell-to-Outside Leakage to Pressure Equalization</u>
32	Cell A to Cell B N ₂ and Na at 900°F	Cell C N ₂ at 600°F
33	Cell B to Cell C N ₂ at 600°F	Cell A O ₂ at 300°F
34	Cell C to Cell D O ₂ at 300°F	Cell A N ₂ at 600°F Cell B N ₂ at 900°F

These three cases use input data cards which describe cell data and which have been checked before. These cases concentrate on checking the input data cards which are used to describe cell-to-cell leakage and cell-to-outside leakage, and these cards are listed below.

High-Pressure Cells	Leak Means	Listed are Card and Card Series Number				
		Low-Pressure Cells				
		Cell A	Cell B	Cell C	Cell D	Outside
Cell A	Nozzle	--	10	20	30	40
	Coefficient	--	11	21	31	41
Cell B	Nozzle	10	--	50	60	70
	Coefficient	11	--	51	61	71
Cell C	Nozzle	20	50	--	80	90
	Coefficient	21	51	--	81	91
Cell D	Nozzle	30	60	80	--	--
	Coefficient	31	61	81	--	--
Outside	Nozzle	40	70	90	--	--
	Coefficient	41	71	91	--	--

Note that Cell D is unique because there is no code input that can define Cell D-to-outside leakage.

3.9.1 Thermodynamic Analysis

This leakage situation and the following thermodynamic analysis were contributed by Ronald D. Gasser of the Brookhaven National Laboratory. These contributions were important to the development of the CACECO Code because they showed that the energy functions used in early versions of the code were defective. Clever code tests such as this leakage situation are encouraged.

The leakage situation assumed by Mr. Gasser had two cells filled with Ideal Gas. The initial conditions of the higher-pressure cell were mass M_{10} , pressure P_{10} and temperature T_{10} and of the lower-pressure cell M_{20} , P_{20} , and T_{20} . Also, $T_{10} = T_{20}$. The pressure equalization of these cells began with leakage from the higher- to the lower-pressure cell. The generalized, open thermodynamic system described by Perry⁽¹⁰⁾ was specialized to this leakage situation by eliminating the heat input, dQ , the work output, dW , the elevation effects, $g z/g_c$, the velocity effects, $v^2/2 g_c$, and the input stream. There remain for the higher-pressure

cell the system of mass M_1 (lb) and unit energy U_1 (Btu/lb) and its output stream of mass increment dM_1 (lb) and unit enthalpy H_1 (Btu/lb):

$$d(M_1 U_1) = H_1 dM_1 \quad (3.9.1)$$

The assumption of constant heat capacity for the material of the system permits the energy and enthalpy functions to be presented in terms of temperature as: $U = C_v T$ and $H = C_p T$. The system equation is then:

$$d(M_1 C_v T_1) = C_v T_1 dM_1 + C_v M_1 dT_1 = C_p T_1 dM_1 \quad (3.9.2)$$

By rearrangement and with $k = C_p/C_v$ (the heat capacity ratio), the equation is as follows:

$$dT_1/T_1 = \frac{C_p - C_v}{C_v} dM_1/M_1 = (k - 1) dM_1/M_1 \quad (3.9.3)$$

This differential equation has the following solution in terms of temperature and mass,

$$T_1 = T_{10} (M_1/M_{10})^{k-1} \quad (3.9.4)$$

and, because of the Ideal Gas Law, $PV = NRT$, the following solution in terms of pressure and mass:

$$P_1 = P_{10} (M_1/M_{10})^k \quad (3.9.5)$$

The lower-pressure cell has the system of mass M_2 , unit energy U_2 , its input stream-of-mass increment dM_1 , and unit enthalpy H_1 :

$$d(M_2 U_2) = H_1 dM_1 \quad (3.9.6)$$

Again, this equation is presented in terms of temperature as follows:

$$d(M_2 C_v T_2) = C_v T_2 dM_2 + C_v M_2 dT_2 = C_p T_1 dM_1 \quad (3.9.7)$$

With constant total mass, $M = M_1 + M_2$, the substitution of Equation 3.9.4 into Equation 3.9.7 leads to the following:

$$dT_2/dM_2 + T_2/M_2 = k (T_{10}/M_2) \left[(M - M_2)/M_{10} \right]^{k-1} \quad (3.9.8)$$

This differential equation has the following solution in terms of temperature and mass:

$$T_2 = T_{20} M_{20}/M_2 + (T_{10} M_{10}/M_2) (1 - P_1/P_{10}) \quad (3.9.9)$$

and the following solution in terms of pressure and mass:

$$P_2 = P_{20} + P_{10} (V_2/V_1)(1 - P_1/P_{10}) \quad (3.9.10)$$

The equalization pressure when leakage ceases is when $P_1 = P_2$ in Equation 3.9.12:

$$P_{\text{equal}} = (V_1 P_{20} + V_2 P_{10}) / (V_1 + V_2) \quad (3.9.11)$$

3.9.2 CACECO Check

These leakage situations for pressure equalization were planned with the following parameters and initial conditions: equal volumes, 10 to 1 atmosphere pressure, and three temperatures.

<u>Item</u>	<u>High-Pressure Cell</u>	<u>Low-Pressure Cell</u>	
Volume, ft ³	<u>1.0 x 10⁶</u>	<u>1.0 x 10⁶</u>	<i>p.B. 84</i>
Initial pressure, psia	P ₁₀ = <u>147.0</u>	P ₂₀ = <u>14.70</u>	
Nitrogen-sodium leakage.			
Initial temperature, °F	T ₁₀ = <u>900.0</u>	T ₂₀ = <u>900.0</u>	<i>p.B. 84</i>
Initial mass, lb N ₂	<u>282,151</u>	<u>28,126</u>	<i>Case 32,</i>
lb Na	<u>84</u>	<u>84</u>	<i>p. 2</i>
lb, total	M ₁₀ = <u>282,235</u>	M ₂₀ = <u>28,210</u>	
Nitrogen-oxygen leakage.			
Initial temperature, °F	T ₁₀ = <u>600.0</u>	T ₂₀ = <u>600.0</u>	<i>p.B. 85</i>
Initial mass, lb N ₂	<u>362,153</u>	<u>36,215</u>	<i>Case 33,</i>
lb O ₂	<u>4</u>	<u>0</u>	<i>p. 2</i>
lb, total	M ₁₀ = <u>262,157</u>	M ₂₀ = <u>36,215</u>	
Oxygen leakage.			
Initial temperature, °F	T ₁₀ = <u>300.0</u>	T ₂₀ = <u>300.0</u>	<i>p.B. 86</i>
Initial mass, lb O ₂	M ₁₀ = <u>577,013</u>	M ₂₀ = <u>57,701</u>	<i>Case 34,</i>
			<i>p. 3</i>

With equal cell volumes and these initial pressures, the equalization pressure of Equation 3.9.13 is 80.85 psia, independent of the heat capacity ratio. The results of hand calculations using Equations 3.9.4, 3.9.5, 3.9.11 and 3.9.12 and the CACECO code results for these debug cases are summarized in Table 3.32. The remarkable agreement between the hand calculations and the CACECO results show that the energy functions used for nitrogen and oxygen are correct.

TABLE 3.32
DEBUG CASES 32, 33 AND 34

<u>Item</u>		<u>Calculated</u>	<u>CACECO Result</u>
<u>Nitrogen-sodium leakage, k = 1.35833</u>			
<i>Case 32, p.14</i>	1. To equalization pressure with $P_1 = P_2$, psia	80.85	<u>80.72</u>
	a. High-pressure cell: Temperature, T_1 , °F Mass, M_1 , lb	701.6 181,745.	699.2 <u>181,831 lb</u> N ₂ 6 lb Na vapor <u>65 lb</u> Na liquid
	b. Low-pressure cell: Temperature, T_2 , °F Mass, M_2 , lb	1,180.1 128,700.	1,179.6 <u>128,445 lb</u> N ₂ 97 lb Na vapor
	2. To outside atmosphere at 14.7 psia		
	a. High-pressure cell: Temperature, T_1 , °F Mass, M_1 , lb	281.0 51,808.	255.7 <u>53,609 lb</u> N ₂ 69 lb Na liquid
<u>Nitrogen-oxygen leakage, k = 1.37464</u>			
<i>Case 33, p.13</i>	1. To equalization pressure with $P_1 = P_2$, psia	80.85	<u>80.64</u>
	a. High-pressure cell: Temperature, T_1 , °F Mass, M_1 , lb	440.7 234,434.	437.8 <u>234,706 lb</u> N ₂ 3 lb O ₂
	b. Low-pressure cell: Temperature, T_2 , °F Mass, M_2 , lb	827.8 163,938	826.0 <u>163,662 lb</u> N ₂ 2 lb O ₂
	2. To outside atmosphere at 14.7 psia		
	a. High-pressure cell: Temperature, T_1 , °F Mass, M_1 , lb	106.1 67,832.	86.6 <u>70,115 lb</u> N ₂ 1 lb O ₂

TABLE 3.32 (continued)
DEBUG CASES 32, 33 AND 34

<u>Item</u>	<u>Calculated</u>	<u>CACECO Result</u>	
<u>Oxygen leakage, k = 1.37216</u>			
1. To equalization pressure with P ₁ = P ₂ , psia	80.85	<u>80.63</u>	<i>Case 34, p.17</i>
a. High-pressure cell:			
Temperature, T ₁ , °F	186.3	<u>183.9</u>	
Mass, M ₁ , lb O ₂	373,223.	<u>373,466.</u>	
b. Low-pressure cell:			
Temperature, T ₂ , °F	462.3	<u>461.0</u>	
Mass, M ₂ , lb O ₂	261,491.	<u>261,248.</u>	
2. To outside atmosphere at 14.7 psia			
a. High-pressure cell:			
Temperature, T ₁ , °F	60.9	<u>54.0</u>	
Mass, M ₁ , lb O ₂	208,948.	<u>211,749.</u>	<i>Case 33, p.13</i>

3.10 DEBUG CASES 35 AND 36, SODIUM RECYCLE

Debug Cases 35 and 36 check the sodium recycle feature of the code. This feature is activated by Card 2100 to transfer sodium pool mass from one cell to another. The transfer is made without regard to cell pressures and temperatures. The transfer is made as if the sodium from the first cell overflowed a dam or weir into the second cell. This feature was provided to the code in order to investigate the following accident scenario:

- 1.) Fission-product decay power and sodium-concrete reaction energy boil sodium from the pool in the reactor cavity.
- 2.) The sodium vapor passes through ducts into an adjacent inert gas cell and condenses on the roof and walls, and
- 3.) The sodium condensate accumulates on the floor of the inert gas cell forming a pool.

The recycle feature permitted the sodium to recycle from the inert gas cell back to the reactor cavity for subsequent reboiling. The overall effect was to maintain sodium and keep the fission products covered in the reactor cavity while spreading the decay power and reaction energy through the concrete structures of the roofs, walls and floors of the cavity and inert gas cell.

These two cases use input data cards which describe cell conditions and a sodium spray and a sodium spill into the cells, all cards which have been checked before. These cases concentrate on checking the operation of the input data on Card 2100.

The plan of Debug Case 35 is summarized as follows:

- 1.) Spray 1300⁰F sodium into Cell A at the rate of 10,000 lb/hr.

- 2.) When 2000 lb of sodium have accumulated in Cell A, overflow further additions into cell B and let it accumulate.
- 3.) Note that the case restart at 0.5 hr can input a different recycle directive on Card 2100.
- 4.) Spill 1000⁰F sodium into cell C at the rate of 10,000 lb/hr.
- 5.) When 7000 lb of sodium have accumulated in Cell C, overflow further additions into cell D and let it accumulate.

The results of Case 35 are shown in Figures 3.23 and 3.24. These results confirm the operation of this recycle feature.

The plan of Case 36 is similar to that of Case 35 except that the sodium sprays into Cell D to overflow into Cell C and that the sodium spills into Cell B to overflow into Cell A. The results confirm the operation of this recycle feature for this case.

FIGURE 3.23. CACECO results for Debug Case 35 with 10,000 lb/hr spray of sodium going into Cell A, which overflows with 2000 lb accumulation into Cell B. At case restart at 0.5 hr, this overflow facility is removed from Cell A and the spray accumulates.

FIGURE 3.24. CACECO results for Debug Case 35 with 10,000 lb/hr spill of sodium going into Cell C, which overflows with 7000 lb accumulation into Cell D.

4.0 REFERENCES

1. R. D. Peak, Users' Guide to CACECO Containment Analysis Code, HEDL-TME 79-22, Hanford Engineering Development Laboratory, Richland, WA, July 1979.
2. H. S. Carslaw and J. C. Jaeger, Conduction of Heat in Solids, 2nd ed., Oxford at the Clarendon Press, 1959.
3. Carslaw and Jaeger, p. 316.
4. R. D. Zerkle and J. E. Sunderland, "The Transient Temperature Distribution in a Slab Subject to Thermal Radiation," J. of Heat Transfer, Trans. Am. Soc. Mech. Eng., Series C, 87, pp. 117-133, 1965.
5. Carslaw and Jaeger, p. 101.
6. J. A. Clark, J. Lammers, M. Kreplin and M. E. Korybalski, "Radioactive Exchange In Multisurfaced Enclosure Systems," Heat Transfer 1974, Proceeding of the Fifth International Heat Transfer Conference, September 3-7, 1974, Tokyo, Japan, The Society of Chemical Engineers, Japan, Vol. 1, pp. 46-50, 1974.
7. J. A. Wiebelt, Engineering Radiation Heat Transfer, Holt, Rinehart and Winston, New York, 1966; Configuration A-3, p. 261; p. 86, p. 90.
8. Weibelt, p. 115.
9. L. C. Richardson, et al, CONTEMPT, A Computer Program for Predicting the Containment Pressure - Temperature Response of a Loss-of-Coolant Accident, IDO-17220, June 1967.
10. R. H. Perry, ed., Chemical Engineers' Handbook, 4th ed., McGraw-Hill Book Company, New York, 1970, pp.4-32.

APPENDIX A

PROPERTY DATA USED INSIDE THE CACECO CODE

Hand calculations to estimate accident effects are made easier when the properties of the various materials are readily available in tables. Also, the hand calculations to check the operation of the CACECO code achieve better agreement with the code results when these calculations use the code property values. Finally, these property values are themselves most easily checked when they are tabulated in convenient form. The properties are tabulated for the following materials:

<u>Material</u>	<u>Energy</u>	<u>Enthalpy</u>	<u>Volume</u>	<u>Pressure</u>	<u>Solubility</u>	<u>Heat of Formation</u>
Carbon	x					
Carbon dioxide	x	x				
Hydrogen	x	x				
Nitrogen	x	x				
Oxygen	x	x				
Sodium	x	x	x	x		
Sodium hydride				x	x	x
Sodium hydroxide	x					
Sodium oxide	x					
Water	x	x	x	x		

PROGRAM CALC (OUTPUT,TAPE6=OUTPUT)

ROY D. PEAK, HEDL, 2-26-77. CHECK ENERGY AND ENTHALPY FUNCTIONS FOR USE IN THE CACECO CODE.

CHECK INTERNAL ENERGY FUNCTIONS FOR CARBON, DISODIUM OXIDE AND SODIUM HYDROXIDE. CORRELATIONS PER JANAF THERMOCHEMICAL TABLES-DOW CHEMICAL COMPANY, AUGUST 1965.

CARBON, C, INTERNAL ENERGY FUNCTION.

UCB(TF) = TF*(+0.205292+TF*(+9.17E-5))

DISODIUM OXIDE, NA2O, INTERNAL ENERGY FUNCTION FOR SOLID.

UNA2O(TF) = TF*(0.27452+TF*4.4278E-5)

SODIUM HYDROXIDE, NaOH, INTERNAL ENERGY FUNCTION FOR LIQUID.

NOTE: MELTING POINT = 606.47 DEG.F, HEAT OF FUSION = 68.4 BTU/LB.

UNAOH(TF) = TF*0.5070

WRITE(6,100)

FORMAT(1H0//35X

	1	2	3	4	5
TEMP.	UCB-C	U-NA2O	U-NAOH	/35X	
DEG.F	BTU/LB	BTU/LB	BTU/LB	)	
1234.	123.56	123.45	123.45		

TF = 0.0

UC = UCB(TF)

UO = UNA2O(TF)

UH = UNAOH(TF)

IF (TF.LT.606.5) UH = UH-68.4

WRITE(6,120) TF,UC,UO,UH

FORMAT(35Y,F7.0,3F9.2)

TF = TF+100.0

IF (TF.LT.2001.0) GO TO 110

STOP

END

	Carbon	Sodium	Sodium
	Energy	Oxide	Hydroxide
	Energy	Energy	Energy
TEMP.	UCB-C	U-NA2O	U-NAOH
DEG.F	BTU/LB	BTU/LB	BTU/LB
0.	0.00	0.00	-68.40
100.	21.45	27.89	-17.70
200.	44.73	56.68	33.00
300.	69.34	86.34	83.70
400.	96.79	116.89	134.40
500.	125.57	148.33	185.10
600.	156.19	180.65	235.80
700.	188.64	213.86	354.90
800.	222.92	247.95	405.60
900.	259.04	282.93	456.30
1000.	296.99	318.80	507.00
1100.	336.78	355.55	557.70
1200.	378.40	393.18	608.40
1300.	421.85	431.71	659.10
1400.	467.14	471.11	709.80
1500.	514.26	511.41	760.50
1600.	563.22	552.58	811.20
1700.	614.01	594.65	861.90
1800.	666.63	637.60	912.60
1900.	721.09	681.43	963.30
2000.	777.38	726.15	1014.00

PROGRAM CALC (OUTPUT,TAPE6=OUTPUT)

```

C
C ROY D. PEAK, HEDL, 2-26-77. CHECK ENERGY AND ENTHALPY FUNCTIONS
C FOR USE IN THE CACECO CODE.
5 C CHECK INTERNAL ENERGY AND ENTHALPY FUNCTIONS FOR CARBON DIOXIDE
C AND HYDROGEN. CORRELATIONS PER O.A.HOUGEN AND K.M.WATSON,
C CHEMICAL PROCESS PRINCIPLES, PART 1, 1943.
C
C CARBON DIOXIDE, CO2, ENTHALPY AND INTERNAL ENERGY FUNCTIONS.
10 HCF(TF) = 20.758+TF*0.04516+UCF(TF)
UCF(TF) = TF*(+0.1564+TF*(+4.588E-5+TF*(-5.786E-9)))
C HYDROGEN, H2, ENTHALPY AND INTERNAL ENERGY FUNCTIONS.
HHF(TF) = 453.06+TF*0.9856+UHF(TF)
UHF(TF) = TF*(+2.4444+TF*(+2.8728E-5+TF*(+1.4238E-8)))
15 C
WRITE(6,100)
100 FORMAT(1H0//35X
1 ,44H TEMP. HCF-CO2 UCF-CO2 HHF-H2 UHF-H2 /35X
2 ,44H DEG.F BTU/LB BTU/LB BTU/LB BTU/LB )
20 C 1234. 123.56 123.45 123.45 123.56
TF = 0.0
110 HC = HCF(TF)
UC = UCF(TF)
HH = HHF(TF)
UH = UHF(TF)
25 WRITE(6,120) TF,HC,UC,HH,UH
120 FORMAT(35X,F7.0,4F9.2)
TF = TF+100.0
IF (TF.LT.2001.0) GO TO 110
30 STOP
END

```

TEMP. DEG.F	Carbon Dioxide		Hydrogen	Hydrogen
	Enthalpy	Energy	Enthalpy	Energy
	HCF-CO2	UCF-CO2	HHF-H2	UHF-H2
	BTU/LB	BTU/LB	BTU/LB	BTU/LB
0.	20.76	0.00	453.06	0.00
100.	41.37	16.09	796.36	244.74
200.	62.86	33.07	1140.32	490.14
300.	85.20	50.89	1485.03	736.29
400.	108.35	69.53	1830.57	983.27
500.	132.28	88.95	2177.02	1231.16
600.	156.96	109.11	2524.48	1480.06
700.	182.35	129.98	2873.02	1730.04
800.	208.41	151.52	3222.74	1981.20
900.	235.11	173.70	3573.71	2233.61
1000.	262.41	196.49	3926.03	2487.37
1100.	290.29	219.85	4279.77	2742.55
1200.	318.70	243.75	4635.03	2999.25
1300.	347.61	268.15	4991.89	3257.55
1400.	376.99	293.01	5350.44	3517.54
1500.	406.80	318.30	5710.75	3779.29
1600.	437.01	343.99	6072.92	4042.90
1700.	467.58	370.05	6437.04	4308.46
1800.	498.47	396.43	6803.17	4576.03
1900.	529.66	423.10	7171.43	4845.73
2000.	561.11	450.03	7541.88	5117.62

PROGRAM CALC (OUTPUT,TAPE6=OUTPUT)

ROY D. PEAK, HEDL, 2-26-77. CHECK ENERGY AND ENTHALPY FUNCTIONS FOR USE IN THE CACECO CODE.

CHECK INTERNAL ENERGY AND ENTHALPY FUNCTIONS FOR NITROGEN AND OXYGEN. DATA FROM JANAF THERMOCHEMICAL TABLES, DOW CHEMICAL COMPANY, AUGUST 1965. DATA CORRELATION OF 12-2-70.

NITROGEN, N2, ENTHALPY AND INTERNAL ENERGY FUNCTIONS.

$HNF(TF) = 32.602 + TF * 0.07092 + UNF(TF)$

$UNF(TF) = TF * (+0.169947 + TF * (+1.65149E-5 + TF * (-1.23100E-9)))$

OXYGEN, O2, ENTHALPY AND INTERNAL ENERGY FUNCTIONS.

$HOF(TF) = 28.543 + TF * 0.06209 + UOF(TF)$

$UOF(TF) = TF * (+0.154581 + TF * (+2.01855E-5 + TF * (-2.15136E-9)))$

WRITE(6,100)

100 FORMAT(1HC//35X

1	.44H	TEMP.	HNF-N2	UNF-N2	HOF-O2	UOF-O2 /35X
2	.44H	DEG.F	BTU/LB	BTU/LB	BTU/LB	BTU/LB)
		1234.	123.56	123.45	123.45	123.56

TF = 0.0

110 HN = HNF(TF)

UN = UNF(TF)

HO = HOF(TF)

UO = UOF(TF)

WRITE(6,120) TF,HN,UN,HO,UO

120 FORMAT(35X,F7.0,4F9.2)

TF = TF+100.0

IF (TF.LT.2001.0) GO TO 110

STOP

END

	Nitrogen Enthalpy	Nitrogen Energy	Oxygen Enthalpy	Oxygen Energy
TEMP. DEG.F	HNF-N2 BTU/LB	UNF-N2 BTU/LB	HOF-O2 BTU/LB	UOF-O2 BTU/LB
0.	32.60	0.00	28.54	0.00
100.	56.85	17.16	50.41	15.66
200.	81.43	34.64	72.67	31.71
300.	106.32	52.44	95.30	48.13
400.	131.51	70.54	118.30	64.92
500.	157.01	88.95	141.66	82.07
600.	182.80	107.65	165.35	99.55
700.	208.88	126.63	189.37	117.36
800.	235.23	145.90	213.70	135.48
900.	261.36	165.43	238.33	153.90
1000.	288.75	185.23	263.25	172.62
1100.	315.90	205.29	288.44	191.60
1200.	343.30	225.59	313.90	210.85
1300.	370.93	246.14	339.60	230.34
1400.	398.81	266.92	365.54	250.07
1500.	426.91	287.92	391.71	270.03
1600.	455.23	309.15	418.08	290.19
1700.	483.76	330.59	444.65	310.55
1800.	512.49	352.23	471.41	331.10
1900.	541.42	374.07	498.33	351.82
2000.	570.55	396.11	525.42	372.69

SATURATION PROPERTIES OF SODIUM USED BY THE CACECO CODE:

0-2000 DEG.F.

TEMP. DEG.F	PRESSURE PSIA	-SPECIFIC VOLUME-		-----ENTHALPY-----			----INTERNAL ENERGY----			AVG. MOLE WEIGHT
		LIQUID FT ³ /LB	VAPOR FT ³ /LB	LIQUID BTU/LB	H.OF.V BTU/LB	VAPOR BTU/LB	LIQUID BTU/LB	E.OF.V BTU/LB	VAPOR BTU/LB	
0.	0.	0.00000	0.	0.00	0.00	0.00	0.00	0.00	0.00	0.00
100.	2.347E-12	.01702	1.113E+14	124.86	2001.04	2125.90	124.86	1952.71	2077.57	22.99
200.	1.119E-09	.01725	2.750E+11	158.32	1988.84	2147.16	158.32	1931.88	2090.20	23.00
300.	1.042E-07	.01750	3.399E+09	239.83	1927.91	2167.74	239.83	1862.37	2102.19	23.01
400.	3.353E-06	.01775	1.193E+08	272.05	1915.07	2187.12	272.05	1841.02	2113.06	23.05
500.	5.203E-05	.01801	8.564E+06	303.75	1901.07	2204.82	303.75	1818.63	2122.38	23.11
600.	4.787E-04	.01824	1.023E+06	335.00	1885.52	2220.52	335.00	1794.86	2129.86	23.21
700.	2.992E-03	.01856	1.782E+05	365.86	1868.26	2234.12	365.86	1769.61	2135.47	23.34
800.	1.393E-02	.01885	4.128E+04	396.42	1849.35	2245.77	396.42	1742.95	2139.36	23.51
900.	5.157E-02	.01915	1.194E+04	426.72	1829.02	2255.74	426.72	1715.12	2141.85	23.70
1000.	1.592E-01	.01946	4.113E+03	456.85	1807.59	2264.44	456.85	1686.45	2143.30	23.93
1100.	4.243E-01	.01978	1.632E+03	486.87	1785.40	2272.26	486.86	1657.26	2144.13	24.17
1200.	1.003E+00	.02011	7.271E+02	516.84	1762.75	2279.59	516.84	1627.83	2144.67	24.42
1300.	2.146E+00	.02046	3.563E+02	546.84	1739.88	2286.72	546.83	1598.38	2145.21	24.69
1400.	4.226E+00	.02082	1.892E+02	576.94	1716.92	2293.86	576.92	1569.02	2145.94	24.96
1500.	7.753E+00	.02119	1.075E+02	607.20	1693.91	2301.10	607.17	1539.78	2146.95	25.24
1600.	1.337E+01	.02157	6.476E+01	637.69	1670.97	2308.66	637.64	1510.79	2148.43	25.52
1700.	2.177E+01	.02197	4.125E+01	668.48	1648.47	2316.94	668.39	1482.36	2150.75	25.80
1800.	3.392E+01	.02234	2.740E+01	699.64	1625.60	2325.24	699.50	1453.78	2153.28	26.09
1900.	5.082E+01	.02281	1.887E+01	731.23	1602.14	2333.37	731.02	1424.89	2155.91	26.40
2000.	7.361E+01	.02326	1.341E+01	763.33	1577.86	2341.19	763.01	1395.50	2158.51	26.73

SODIUM HYDRIDE DATA USED BY THE CACECO CODE, 0-2000 DEG.F.

TEMP. DEG.F	HYDROGEN PRESSURE PSIA	NAH SOLUBILITY LB-NAH/LB-NA	SODIUM HYDRIDE HEAT OF FORMATION BTU/LB-NAH
0.	1.019E-14	1.015E-10	1112.66
100.	1.957E-10	1.323E-08	1102.81
200.	1.889E-07	3.938E-07	1092.95
300.	2.987E-05	4.799E-06	1083.09
400.	1.454E-03	3.269E-05	1073.23
500.	3.150E-02	1.493E-04	1063.38
600.	3.819E-01	5.117E-04	1053.52
700.	3.011E+00	1.418E-03	1043.66
800.	1.710E+01	3.344E-03	1033.81
900.	7.523E+01	6.950E-03	1023.95
1000.	2.702E+02	1.307E-02	1014.09
1100.	8.235E+02	2.266E-02	1004.24
1200.	2.195E+03	3.676E-02	994.38
1300.	5.232E+03	5.646E-02	984.52
1400.	1.136E+04	8.279E-02	974.66
1500.	2.279E+04	1.168E-01	964.81
1600.	4.274E+04	1.593E-01	954.95
1700.	7.561E+04	2.111E-01	945.09
1800.	1.272E+05	2.729E-01	935.24
1900.	2.047E+05	3.451E-01	925.38
2000.	3.169E+05	4.283E-01	915.52

PROPERTIES OF WATER USED BY THE CACECO CODE, 0-2000 DEG.F.

TEMP. DEG.F	PRESSURE PSIA	-SPECIFIC VOLUME-		-----ENTHALPY-----			-----INTERNAL ENERGY-----		
		LIQUID FT3/LB	VAPOR FT3/LB	LIQUID BTU/LB	H.OF.V BTU/LB	VAPOR BTU/LB	LIQUID BTU/LB	E.OF.V BTU/LB	VAPOR BTU/LB
0.	0.	0.00000	0.	0.00	0.00	0.00	0.00	0.00	0.00
100.	9.513E-01	.01614	3.493E+02	67.91	1037.37	1105.29	67.91	975.90	1043.81
200.	1.152E+01	.01672	3.373E+01	168.14	975.81	1143.96	168.11	903.95	1072.06
300.	6.703E+01	.01730	6.433E+00	269.53	914.25	1183.78	269.31	834.68	1103.99
400.	1.470E+01	.01730	3.447E+01	315.58	914.25	1229.83	315.53	823.48	1139.02
500.	1.470E+01	.01730	3.853E+01	362.55	914.25	1276.80	362.50	812.45	1174.95
600.	1.470E+01	.01730	4.258E+01	410.41	914.25	1324.66	410.36	801.42	1211.79
700.	1.470E+01	.01730	4.663E+01	459.17	914.25	1373.42	459.12	790.39	1249.51
800.	1.470E+01	.01730	5.068E+01	508.80	914.25	1423.05	508.75	779.36	1288.11
900.	1.470E+01	.01730	5.473E+01	559.29	914.25	1473.54	559.24	768.33	1327.58
1000.	1.470E+01	.01730	5.879E+01	610.64	914.25	1524.89	610.59	757.30	1367.89
1100.	1.470E+01	.01730	6.284E+01	662.82	914.25	1577.07	662.78	746.27	1409.05
1200.	1.470E+01	.01730	6.689E+01	715.84	914.25	1630.09	715.79	735.24	1451.04
1300.	1.470E+01	.01730	7.094E+01	769.67	914.25	1683.92	769.63	724.21	1493.84
1400.	1.470E+01	.01730	7.499E+01	824.31	914.25	1738.56	824.27	713.18	1537.45
1500.	1.470E+01	.01730	7.905E+01	879.75	914.25	1794.00	879.70	702.15	1581.85
1600.	1.470E+01	.01730	8.310E+01	935.96	914.25	1850.21	935.91	691.12	1627.04
1700.	1.470E+01	.01730	8.715E+01	992.95	914.25	1907.20	992.90	680.09	1672.99
1800.	1.470E+01	.01730	9.120E+01	1050.69	914.25	1964.94	1050.64	669.06	1719.71
1900.	1.470E+01	.01730	9.525E+01	1109.18	914.25	2023.43	1109.14	658.03	1767.17
2000.	1.470E+01	.01730	9.931E+01	1168.41	914.25	2082.66	1168.36	647.00	1815.37

APPENDIX B

CACECO CODE INPUT DATA FOR THE DEBUG CASES

The enclosed microfiche lists the CACECO Code input data for all 36 of the debug cases described in this validation report. Each case is independent of the others and can be run separately. Most of the cases have comment cards and comments to explain special features and expected results.

DISTRIBUTION

UC 79p (276)

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J. P. Hale	W/C-76
T. A. Mangelsdorf	W/B-63
H. C. Martin	W/C-76
W. J. McShane	W/B-12
L. D. Muhlestein	W/221T
A. Padilla, Jr.	W/F-126C
R. D. Peak (2)	W/C-75
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W. F. Sheely	W/C-44
D. E. Simpson	W/C-80
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