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FFTF SODIUM FIRES
AND BLAST ANALYSIS STUDY

ATOMICS INTERNATIONAL

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AND BLAST ANALYSIS STUDY**

By

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I. SUMMARY

A. OBJECTIVE

The objective of this interim study is to provide pressure and temperature data for two reference reactor hot cell arrangements (the rectangular cell and the alternate)* and for two atmospheres (air and inert) under Design Basis Accident (DBA) and sodium fire conditions.

B. PURPOSE

The determination of the maximum pressure and temperature in the reactor hot cell for the specified major accident conditions for two hot cell atmospheres and for two hot cell configurations will provide a basis for selecting the configuration, atmosphere, and design pressure criteria for the hot cell. Data on the decay rates of pressure and temperature in the hot cell for the various accidents as a function of hot cell leakage rate, coupled with information on the spatial and temporal distribution of PuO_2 and radionuclides will provide a basis for evaluating the leak tightness requirements of the hot cell. Pressure and temperature decay rate data as a function of hot cell leakage will also provide the pressure-temperature-time characteristics of the outer containment for evaluating leakage requirements and site radiological dose.

This study will also provide information required to evaluate the magnitude of reduction of hot cell pressure loading by venting into adjacent volumes.

C. ACCIDENT SPECIFICATION

The following accident conditions were specified by PNL⁽¹⁾ for this study:

- 1) A large spill of 20 tons of sodium on the hot cell floor (pool fire),
- 2) DBA expulsion of 20 tons of sodium above the reactor core into the hot cell,
- 3) Sodium sprayed into the hot cell at the rate of 1000 lb/min for 10 min due to a nozzle or jumper leak,
- 4) Venting of DBA-vaporized fuel into the hot cell or the reactor vessel cavity, superimposed upon the expulsion of 20 tons of sodium,

*The "alternate" hot cell is a cylindrical hot cell.

- 5) Venting of pressure generated in the hot cell after C-4, into the primary heat transfer equipment cells, and into reactor vessel cavity, and
- 6) Pressure buildup in the outer containment due to leakage at specified rates from the hot cell following certain accidents.
- 7) Accidents 1 through 4 in the outer containment only, and absence of a hot cell structure being assumed.

The initial sodium temperature for the above cases were specified to be 700°F; however, the effect of increasing this temperature to 1200°F was evaluated for some cases.

D. METHOD

The pressures and temperatures generated during a sodium pool fire were obtained by using the SOFIRE code developed at AI, see Appendix A and Section IV-A.

The adiabatic pressure and temperature in the hot cell (or outer containment) due to the instantaneous reaction of expelled sodium with air was obtained by computing the chemical equilibrium by a free energy minimization technique available in the ANL Chemical Equilibrium Calculations Program.^(6,7)

The pressure-and-temperature history during the nozzle spray fire was obtained by using the TAP (Thermal Analyzer Program) code⁽³⁾ which computes heat transfer from the gas to the containment structure in the presence of an energy source term during the spraying period. The energy source term is derived from the code described in the paragraph above.

The equilibration of pressure in the hot cell and reactor vessel during the venting of vaporized fuel (or during venting of hot cell pressure to adjacent volumes) was computed on the basis of the adiabatic expansion of an ideal gas between two interconnected volumes, and on instantaneous mixing of fuel vapor and hot cell gas. This calculation is programmed for computer solution in the PEQUIB I code developed at AI, see Appendix C and Section IV-C.

The decay of the maximum temperature and pressure after DBA venting to the hot cell (or outer containment) or hot cell venting to other volumes was computed with the TAP code.

The pressure buildup in the outer containment as a result of hot cell leakage during several accidents was computed with a simple code, CELLEAK, written for this purpose. The code is based on a mass balance, the ideal gas law, and on assumed relationships between leakage pressure differential and the design leak rate.

E. CONCLUSIONS

The maximum pressure rise generated in the FFTF hot cells for the range of accident conditions and hot cell atmospheres studied is estimated to vary from 3 psig (pool fire in the inerted alternate cell) to 112 psig (DBA and sodium expulsion in rectangular cell) for an initial sodium temperature of 700°F. An increase in the initial sodium temperature to 1200°F for the worst accident conditions (DBA and sodium expulsion) results in an increase in the maximum pressure of 10% and 40% for hot cell with an air atmosphere, and with an inert atmosphere, respectively. For any given accident, the pressure generated in the rectangular hot cell is higher than that in the cylindrical hot cell.

A reduction in the assumed quantity of sodium expelled by the DBA, in the molar ratio range of interest to the present study, does not lead to proportionately lower maximum theoretical pressures; e.g., a reduction in sodium expelled from 20 to 5 tons would only result in an ~30% reduction in theoretical pressure.

The assumption that a large quantity of DBA-expelled sodium dispersed finely enough to react instantaneously and in equilibrium with all of the available oxygen in the hot cell is difficult to justify; hence, the maximum theoretical pressure estimated is very conservative. One anticipates that the maximum pressure will be between those for the pool fire and the sodium expulsion case.

The mitigative effectiveness of the use of an inert atmosphere in the hot cell is clearly demonstrated. The use of adjacent venting volumes to reduce the pressure in the hot cell during the DBA appears to be worthwhile provided the venting area is increased substantially.

The pressure buildup in the outer containment due to leakage from the hot cell is relatively small, amounting to less than 2 psig for the worst hot cell accident.

The maximum pressures generated in the outer containment, in the absence of the hot cell, for the equivalent accidents would range from 22 to 67 psig.

II. INTRODUCTION

One of the concepts under consideration for FFTF refueling involves the use of a hot cell which is located over the reactor vessel and within the outer containment. In the event of a loss of integrity of the reactor top shield plug due to the DBA, the refueling hot cell becomes a part of the inner containment barrier. It is, of course, also the inner containment barrier for accidents such as sodium-pool and spray fires which may be postulated during certain shutdown operations such as during loop maintenance. Of direct interest to the designer, is the magnitude of pressure generated in the hot cell during an accident. The hot cell configurations being considered include a rectangular one and an alternate concept having a cylindrical geometry.

In this study, we have made estimates of the pressures and temperatures generated for a range of accident conditions postulated for the FFTF. The hot cell atmosphere was considered to be either air or inert (2 v/o O₂). The conditions that exist when the hot cell is vented to adjacent volumes is also examined. In addition, the consequences with respect to the outer containment have been evaluated for the same range of accidents, in the absence of the hot cell.

III. ACCIDENT CONDITIONS

The various initial conditions and assumed accidents presented below were specified by PNL⁽¹⁾ for this study. These are postulated accidents having initiating mechanisms and sequential events whose description is beyond the scope of the present study and therefore will not be treated here. The DBA conditions used for this study are preliminary data provided by BNW at the initiation of the study and are not to be interpreted as the DBA for the facility. The conditions used, however, are considered to be a conservative representation of the maximum energy release from postulated nuclear excursions resulting from hypothetical accidents terminated by disassembly of the reactor core.

A. CONTAINMENT CONFIGURATION

The containment system for the FFTF for this study is shown on Building Plan SVIII Drawings SK-3-12968 through SK-3-12980.⁽²⁾ Two refueling hot cell concepts were considered in this study, the rectangular hot cell shown in Figure 1, and an alternate hot cell, cylindrical in shape (not shown in the above-referenced drawings). The pertinent characteristics of the various portions of the containment system, based upon References 1 and 2, are shown in Table 1.

B. ACCIDENTS

1. Sodium Pool Fires

- a) Sodium is expelled from reactor in spills of 10 and 20 tons at 700°F on the hot cell floor; air and inert atmospheres in the cell.
- b) Spills similar to (1a) above, on the main operating floor, without a hot cell (air atmosphere in outer containment only).
- c) Several calculations were made for an initial sodium temperature of 1200°F.

2. Sodium Spray Fires

- a) Sodium at 700°F is sprayed into the hot cell (air atmosphere only) from a jumper or nozzle leak at the rate of 1000 lb/min for 10 min.

TABLE 1
FFTF CONTAINMENT CHARACTERISTICS

Characteristic	Rectangular Hot Cell	Cylindrical Hot Cell	Outer Containment	Reactor Vessel Cavity	Primary Equipment Cells
Net volume (ft ³)	410,000	239,000	2 x 10 ^{6a} 2.2 x 10 ^{6b}	30,000	180,000
Height (ft)	75	90	-	42	-
Diameter (ft)	50 x 110	60	190	36	-
Wall thickness (ft)	5	5	5/1 ^e	-	-
Roof or head thickness (ft)	5	5	1	-	-
Floor thickness (ft)	8	8	8	-	-
S.S. liner thickness (in.)	3/8	3/8	-	-	-
Initial atmosphere	Air + Inert ^c	Air + Inert ^c	Air	Inert ^c	Inert ^c
Initial cell conditions { Temperature (°F) (in. H ₂ O)	80 100	80 100	80	100	100
	0.5 0.5	0.5 0.5	-	-	-
Pool fire area (ft ²)	5500	2810	12,600	-	-
Wall surface area (ft ²)	29,500	21,600	72,800	-	-
Heat absorbing mass ^d (lb)	1.31 x 10 ⁶	1.31 x 10 ⁶	1.31 x 10 ⁶		

a = Net volume with rectangular hot cell

b = Net volume with cylindrical hot cell

c = Nitrogen with oxygen content ≤2 vol %

d = (1) gas fuel handling cask with shielding, 175 tons; +
 (2) sodium fuel handling cask with shielding, 175 tons; +
 (3) transporter-indexer for 1 and 2 above, 35 tons; +
 (4) secondary gamma shield, 12 tons; +
 (5) nozzle preparation equipment, 60 tons; +
 (6) hot cell bridge crane, 200 tons;
 Total - 657 tons.

e = The Outer Containment = the portion of the 1-ft thick steel-and-concrete containment vessel above the 65-ft elevation, the 5-ft thick floor at the 65-ft elevation, and the 5-ft thick vertical portion of the Primary Heat Transfer Equipment Cell between the 65- and 35-ft elevations.

SCOPE

Figure 1. FFTF Rectangular Hot Cell

AI-68-MEMO-127

- b) Similar to 2a but sprayed directly into the outer containment, without a hot cell.
- c) Expulsion of 20 tons of 700°F* sodium from the reactor into the hot cell with an air atmosphere, as a result of the DBA.

3. Design Basis Accident (DBA)

The characteristics of the DBA are summarized below.

- a) Energy release: 1500 Mw-sec work
- b) Fuel vaporized:
 - 1) Reactor subcritical: 40 lb at 5700°K and 135 atm
 - 2) After explosive disassembly: 800 lb[†]
- c) Assumptions
 - 1) Slow propellant-type energy release, in the form of gas-bubble overpressure, no shock wave
 - 2) Neglect reactor vessel containment potential
 - 3) Venting from reactor vessel either to hot cell or reactor cavity, but not simultaneously
 - 4) Neglect effect of gamma shield.

4. Venting

- a) Venting of the high-pressure, DBA-vaporized fuel into the hot cell immediately follows the expulsion of 20 tons of sodium from the reactor vessel; calculations were made for both air and an inert atmosphere in the cell. The initial sodium temperature was 700°F. §
- b) Fuel vapor venting after the DBA into the reactor vessel cavity but with no path to the hot cell
- c) Venting of the hot cell pressure generated in 4(a) into the lower cavity and primary heat transfer equipment cells, combined

*A few 1200°F cases were evaluated.

†The fuel pressure, temperature, and volume associated with this fuel vapor mass were determined from the fuel equation of state.

§A few 1200°F cases were evaluated.

d) The venting area between the reactor vessel cavity and the equipment cells is 5 ft²

e) The venting area between the reactor vessel cavity and the hot cell is 5 ft².

A summary description of the accidents included in this study is presented in Table 2.

TABLE 2
FFTF SODIUM FIRES AND BLAST ANALYSIS
ACCIDENT SUMMARY

Accident Condition	Description	Sodium (tons)	Initial Sodium Temperature (°F)	Structure	Cell Atmosphere	Fuel
A	Large sodium spill on H. C. floor (pool fire)	10 20	700 1200	Hot cell	Air/Inert	No
B	Expulsion of plenum sodium by DBA into H. C. (explosive spray fire)	20	700 1200	Hot cell	Air/Inert	No
C	Sodium sprayed into H. C. from jumper or nozzle leak	5 (1000 lb/min for 10 min)	700	Hot cell	Air	No
D	Item B and DBA venting to H. C.	20	700 1200	Hot cell	Air/Inert	800 lb Fuel vapor
E	DBA venting to reactor vessel cavity	20	700 1200	Reactor vessel cavity	Inert	800 lb Fuel vapor
F	Item D venting to equipment cells and reactor cavity		700	H. C., cavity and equipment cells	Inert	-
G	Leakage to outer containment after condition C, D, and F	-	-	Outer containment	Air	No
H	Expulsion of reactor sodium by DBA into outer containment	20	700	Outer containment	Air	No
I	Large sodium spill on operating floor	10 20	700	Outer containment	Air	No
J	Sodium sprayed into outer containment from nozzle leak	5 (1000 lb/min for 10 min)	700	Outer containment	Air	
K	Item H and DBA venting to outer containment	20	700	Outer containment	Air	800 lb Fuel vapor

IV. CALCULATION METHODS

A. SODIUM POOL FIRES

The analytical model used for large sodium pool fire analysis is composed of a series of equations, based on an energy and mass balance employed to calculate the energy and gas flows resulting from the fire within a cell. These equations are programmed in the SOFIRE I code for calculation by digital computer to give temperatures, gas flow rates, sodium burning rates, and cell and secondary volume pressures as a function of time.

The geometric model used in the calculations consists of a cell in which the sodium fire is located, and a secondary volume which is connected to the cell by an opening. For the FFTF calculations, a closed system was employed whereby the secondary volume represents the upper half of the system volume. A typical SOFIRE I case representation is shown in Figure 2.

Fixed input conditions to the code include the fire and facility geometries, and the atmospheric conditions outside the building. The wall material thermal properties are chosen to be independent of temperature. Variable conditions which require initial input values include gas and wall temperatures, oxygen concentrations, and initial sodium pool and flame temperature.

During each chosen time increment, the computer calculates (1) the sodium burning rate, which is directly dependent on the oxygen concentration within the system at that time point, (2) the temperature of the sodium flame and the heat transferred from the flame to the system gas or downward to the sodium pool, (3) the heat transferred from the system atmosphere to the walls, (4) the sodium node temperatures based on a heat balance on the input heat from the flame and that lost to the floor, and (5) gas densities and pressure, and the respective oxygen concentration based on the sodium burning rate established at that time. Checks are made throughout the calculation series to determine if all of the sodium is consumed, if the available oxygen has been depleted, or if the bulk sodium temperature has fallen below a temperature which can no longer sustain burning conditions. Each of these checks, if satisfied, may terminate the calculation series. The basic equations used in the SOFIRE I code are presented in Appendix A.

Figure 2. Typical FFTF SOFIRE Configuration

B. ADIABATIC EQUILIBRIUM SODIUM-AIR REACTION

Accident condition B in Section III specifies that 20 tons of sodium above the reactor core is expelled into the hot cell (or outer containment for accident H) with an air atmosphere. It is assumed that 20 tons of sodium at an initial temperature of 700°F (or 1200°F) mixes and reacts immediately with available oxygen in the hot cell. Adiabatic reaction and chemical equilibrium between the various species present are assumed. The only species considered were Na(l), Na(g), NaO(g), Na₂O(s), O₂(g), and N₂. The method for performing these calculations are presented in Appendix B.

C. FUEL VAPOR VENTING INTO HOT CELL AFTER DBA

Accident Condition D, Section III, assumes that the expulsion of sodium (Condition B) into the hot cell and the reaction of the sodium with oxygen is followed immediately by the venting of vaporized fuel from the reactor into the cell.

The basic assumptions underlying these calculations is that immediately upon entering the hot cell, there is a complete and instantaneous mixing between the fuel vapor and the hot cell gas, and that no heat transfer to the containment walls is taking place during that time. Figure 3 shows a schematic of the physical model used in deriving the basic venting equations. These equations are described in Appendix C.

Figure 3. Schematic of Physical Model for Fuel Vapor Venting

D. PRESSURE AND TEMPERATURE DECAY IN CELL DUE TO HEAT TRANSFER TO WALLS

Figure 4 is a schematic of the physical model employed for calculating the pressure and temperature decay histories in the hot cell after all of the accidents except the pool fires. The cell contains a mixture of ideal gas of some known composition, temperature, and pressure. At a given time, heat transfer to the walls is initiated, and it is required to determine the pressure and temperature change of the mixture. The assumptions and equations are discussed below.

Figure 4. Schematic of Physical Model for
Calculating Pressure and Temperature
Change of Gas in Cell

1. Assumptions

- 1) The gas obeys the perfect gas law.
- 2) The temperature and pressure are uniform throughout the gas space.
- 3) The heat transfer coefficients between the gas and the inside containment wall are $2 \text{ Btu/ft}^2\text{-hr}$.
- 4) The thermal diffusivity of the walls is temperature-independent.
- 5) Condensation of species (e.g., sodium) on cooling is neglected.
- 6) Heat flow through the walls is unidirectional.

2. Equations

- 1) Gas mixture,

$$M\bar{C}_v \left(\frac{dT_g}{dt} \right) = - h_i A_i (T_g - T_{w,x=0}), \quad \dots (1)$$

with boundary conditions of:

$$t = 0, \quad T_g = T_{g,o}, \quad \text{and} \quad P_g = P_{g,o} ;$$

the pressure equation is:

$$P_g = P_{g,o} \left(\frac{T_g}{T_{g,o}} \right). \quad \dots (2)$$

2) Wall,

$$\frac{\partial T_w}{\partial t} = \left(\frac{K}{\rho C_p} \right) \frac{\partial^2 T_w}{\partial x^2}, \quad \dots (3)$$

with boundary conditions of:

$$x = 0, \quad -k \frac{\partial T_w}{\partial x} = h_i (T_g - T_{w,x=0}) \quad \text{and}$$

$$x = L, \quad -k \frac{\partial T_w}{\partial x} = h_o (T_{w,x=L} - T_o) .$$

For Equations 1, 2, 3, and Figure 4:

M = total mass of the gaseous mixture,

$\bar{C}_v$ = average specific heat of gaseous mixture at constant volume,

T_g = temperature of the gas,

t = time,

X = location into wall,

P_g = pressure of the gas,

h_i = heat transfer coefficient, gas-wall,

A_i = internal surface area of cell,

T_w = temperature of the wall,

$\bar{J}(g)$ = gaseous species such as fuel or sodium

T_o = temperature of surroundings,
 h_o = heat transfer coefficient, wall + surroundings,
 C_p = specific heat of concrete wall,
 K = thermal conductivity of concrete wall, and
 ρ = density of concrete wall.

The heat content of the gaseous mixture is averaged with respect to the mass of the individual species as follows:

$$\bar{C}_v(T_g) = \frac{(MC_v)_{O_2} + (MC_v)_{N_2} + (MC_v)_J}{M_{O_2} + M_{N_2} + M_J} \quad \dots (4)$$

Equations 1 to 4 were programmed for solution on a digital computer, by use of the TAP code.⁽³⁾ The wall thickness was divided into 16 nodes, and the gas space was treated as one node. Nodes 2 to 12 were spaced in intervals of 0.02 ft. Nodes 12 to 17 were divided equally along the remaining thickness of the wall. The wall thickness employed in the calculations was the average thickness of the entire containment with respect to the surface area.

E. SODIUM NOZZLE SPRAY FIRE

Two of the accident conditions specified in Section III involved the spraying of sodium (resulting from a nozzle or jumper leak) into the hot cell (Accident C) or in the case of no hot cell, directly into the outer containment. For these calculations, Equation 1 was modified to include an energy source term on the right hand side of the equation. This term was obtained by taking the available energy for the reaction of all of the total quantity of sodium sprayed) as calculated according to the method in Section IV-B, and dividing it by the spraying time to obtain the energy source rate, while the gas is simultaneously transferring some of this energy to the containment structure.

F. LEAKAGE FROM HOT CELL TO OUTER CONTAINMENT

For several of the accident conditions (C, D, and F) specified in Section III, calculations were required to determine the pressure and temperature history

in the outer containment vessel resulting from leakage from the hot cell due to the pressures generated.

The geometry of interest for these calculations is shown in Figure 5; subscript "1" refers to the cell, and "2" to the building. The quantities P, T, n, and V refer to pressure, temperature, moles, and volume, respectively.

The quantity L is the fractional leakage rate and is defined by the equation

$$L = \frac{1}{n_1} \left(\frac{dn_1}{dt} \right) . \quad \dots (5)$$

One may write the gas laws for the two compartments:

$$P_1 V_1 = n_1 R T_1 , \quad \text{and} \quad \dots (6)$$

$$P_2 V_2 = n_2 R T_2 . \quad \dots (7)$$

The leakage, L, is known to be a function of the pressure differential ($P_1 - P_2$). Depending on the nature of the leakage paths one may write

$$L = k(P_1 - P_2) \quad \text{or} \quad L = k(P_1 - P_2)^{1/2} .$$

A plot of L vs ($P_1 - P_2$) for the two possibilities is shown in Figure 6. Ordinarily, buildings and structures have a specified design leakage rate, L_d , for a stated pressure, $P_1 = P_d$. Thus, one may rewrite the expressions for L as

$$L = L_d \left[\frac{P_1 - P_2}{P_d - P_2} \right] ,$$

or

$$= L_d \left[\frac{P_1 - P_2}{P_d - P_2} \right]^{1/2} .$$

As a conservative measure, one may assume that the leakage, L, is to be taken as the larger of the two possibilities presented. This is indicated by the

Figure 5. Schematic for Calculating Hot Cell Leakage to Outer Containment

Figure 6. Dependence of Leakage on Pressure Differential

cross-hatching on the curves yielding the higher values. On this basis, one finally adopts the following expressions for L:

$$\begin{aligned}
 L &= L_d \left[\frac{P_1 - P_2}{P_d - P_2} \right]^{1/2}, \quad P_2 \leq P_1 \leq P_d; \text{ and} \\
 &= L_d \left[\frac{P_1 - P_2}{P_d - P_2} \right]; \quad P_1 > P_d.
 \end{aligned}
 \tag{8}$$

The quantity that one wishes to compute is the number of moles leaked, n_L , given given by

$$n_L = n_1(0) - n_1(t);$$

or the fraction leaked

$$\frac{n_L}{n_1(0)} = 1 - \frac{n_1(t)}{n_1(0)}.$$

It is assumed that the thermal exchange between the cell and building is not sufficient to alter T_2 , which is then taken as a constant. Thus, one may write

$$\frac{P_2(t)}{P_2(0)} = \frac{n_2(t)}{n_2(0)} \tag{9}$$

Thus, a system of 5 equations is available, corresponding to the 5 variables: P_1 , n_1 , L , P_2 , and n_2 . The initial conditions in both cell and building are assumed to be known, and the temperature profile in the cell, $T_1(t)$, is assumed to be known. Equations 5 through 9 were programmed for the digital computer for the required calculations.

V. RESULTS AND DISCUSSION

A. HOT CELL CONTAINMENT

1. Sodium Pool Fires

Calculations were performed to determine the pressure and temperature vs time resulting from 10- and 20-ton sodium spills for each hot cell and cell atmosphere by using the SOFIRE code described in Section IV-A. The results for the 10-ton pool fires for 700°F sodium are presented in Figures 7 through 10; a summary of the results is given in Table 3. These results show that the maximum pressures estimated for the alternate or cylindrical hot cell are lower than for the rectangular hot cell. This is due to the larger wall surface area, fire area ratio in the cylindrical hot cell compared with that of the rectangular cell. Comparison of the results in Table 3 for the 20- and 10-ton spills shows somewhat lower temperature and pressures for the 20-ton spill. This is due to the fact that peak pressure occurs early and is not affected by the quantity of sodium. The larger spill does provide a greater heat sink for some of the combustion energy and leads to a lower energy release to the gas. The mitigating effect of a low oxygen atmosphere in the cell is clearly demonstrated in Table 3, for the inert cases.

TABLE 3
SUMMARY OF SODIUM POOL FIRES RESULTS
(700°F Sodium)

Rectangular Hot Cell				Alternate Hot Cell				Sodium Quantity (tons)
Air		Inert		Air		Inert		
P _{max} [*]	T _{max} [†]	P _{max}	T _{max}	P _{max}	T _{max}	P _{max}	T _{max}	
24.8	1000	4.1	251	18.7	863	2.8	202	10
26.8	1150	4.3	259	21.7	950	3.0	208	20

*P = pressure rise in psig

†T = temperature in °F

Figure 7. Sodium Pool Fire in Rectangular Hot Cell,
10-Ton Spill, Air

Figure 8. Sodium Pool Fire in Rectangular Hot Cell,
10-Ton Spill, Inert

Figure 9. Sodium Pool Fire in Cylindrical Hot Cell, 10-Ton Spill, Air

Figure 10. Sodium Pool Fire in Cylindrical Hot Cell, 10-Ton Spill, Inert

2. Sodium Expulsion

The maximum pressure and temperature in the hot cell for expulsion of 20-tons of sodium (700°F) into an air atmosphere (Accident B) was obtained according to the method described in Section IV-B. The results obtained are summarized below. The pressures and temperatures obtained for the case of an inerted hot cell, see Appendix B-2, were part of the Accident D calculation, but are also shown below for comparison with those in air.

Cell Atmos	Rectangular Hot Cell		Cylindrical Hot Cell	
	P _{max} (psig)	T _{max} (°F)	P _{max} (psig)	T _{max} (°F)
Air	111	2430	93	1930
Inert	20.6	890	18.8	812

Calculations of this type were made during the study for other sodium/oxygen molar ratios for the various containment volumes involved. As a result, a plot of theoretical adiabatic, equilibrium pressure due to the sodium-air reaction vs sodium/oxygen ratio was obtained as shown in Figure 11, for an initial sodium temperature of 700°F. Figure 11 also shows the abscissa in terms of the quantity of sodium expelled for the various containment structures. Thus, the maximum pressure due to expulsion of any quantity of sodium in a given structure can be estimated by use of Figure 11. Figure 11 also indicates that even with substantial reductions in the assumed quantity of DBA-expelled sodium, the maximum theoretical pressure in the hot cell is at a substantial level.

3. Sodium Nozzle Spray Fire

The pressure and temperature history of the hot cell (air atmosphere) as result of the spraying of 700°F sodium at 1000 lb/min for 10 min due to a nozzle or jumper leak (Accident C) was determined according to Section IV-E. The results in each of the hot cell concepts is shown in Figures 12 and 13 and in Table 4 (Case 6 and 7).

Figure 11. Maximum Theoretical Pressure vs Quantity of Sodium Expelled in Different Structures (700°F Sodium)

Figure 12. Gas Pressure and Temperature History, Nozzle Spray Fire (Rectangular Hot Cell)

Figure 13. Gas Pressure and Temperature History, Nozzle Spray Fire (Cylindrical Hot Cell)

Case	Cell	Time (hr)	Cell Atmosphere	Pressure (psia)	Temperature (°F)	Change of Condition	Accident Condition
1	Rect Hot Cell	0	Air	14.7	80	Original	-
		0	0.49 N ₂ * 0.51 Na(g)	126(138)	2430(2720)	Sodium-air reaction	B
		4.35 x 10 ⁻⁷	0.49 N ₂ 0.51 Na(g) + fuel†	127(139)	2443(2733)	DBA fuel vapor venting	D
		25	0.49 N ₂ 0.51 Na(g) + fuel†	24§	91	Heat transfer to walls	-
2	Rect Hot Cell	0	Inert	14.7	100	Original	-
		0	N ₂	35.3(44)	890(1227)	Sodium +2% O ₂ reaction	B
		7.1 x 10 ⁻⁷	N ₂ + fuel†	37.4(46.5)	921(1258)	DBA fuel vapor venting	D
		17.2	N ₂ + fuel†	14.65	80	Heat transfer to wall	-
3	Alt Hot Cell	0	Air	14.7	80	Original	-
		0	0.52 N ₂ 0.48 Na(g)	107.5	1930	Sodium-air reaction	B
		4.72 x 10 ⁻⁷	0.52 N ₂ 0.48 Na(g) + fuel†	109.0	1955	DBA fuel vapor venting	D
		25	0.52 N ₂ 0.48 Na(g) + fuel†	24.2	90	Heat transfer to walls	-
4	Alt Hot Cell	0	Inert	14.7	100	Original	-
		0	N ₂	33.6(43.8)	812(1202)	Sodium +20% O ₂ reaction	-
		7.25 x 10 ⁻⁷	N ₂ + fuel†	35.8(45.8)	966(1356)	DBA fuel vapor venting	-
		16.4	N ₂ + fuel†	14.65	79	Heat transfer to walls	-
5	Reactor Cavity	0	Inert	14.7	100	Original	E
		0	N ₂	31	732(1217)	Sodium +2% O ₂ reaction	-
		6.85 x 10 ⁻⁵	0.74 N ₂ 0.26 fuel	44.5(58)	1140(1625)	DBA fuel vapor venting	-
		13.5	0.74 N ₂ 0.26 fuel	15	79	Heat transfer to walls	-
6	Rect Hot Cell	0	Air	14.7	80	Original	-
		0.14	N ₂ + Na(g)	59	1340	Maximum condition during nozzle spray fire	C
		25	N ₂ + Na(g)	15	87	Heat transfer to walls	-
7	Alt Hot Cell	0	Air	14.7	80	Original	-
		0.15	N ₂ + Na(g)	56.3	1240	Maximum condition during nozzle spray fire	C
		25	N ₂ + Na(g)	15.3	93	-	-
8	Rect Hot Cell	0	Air	14.7	80	Original	-
		0	0.49 N ₂ 0.51 Na(g)	128.7	2480	Sodium-air reaction	B
		4.35 x 10 ⁻⁷	0.49 N ₂ 0.51 Na(g) + fuel†	130	2493	DBA fuel vapor venting	D
		3.26 x 10 ⁻³	0.49 N ₂ 0.51 Na(g) + fuel†	95.5	2235	Venting to equip cell and cavity	F
		25	0.49 N ₂ 0.51 Na(g) + fuel†	19.1	87	Heat transfer to walls	-
9	Rect Hot Cell	0	Inert	14.7	100	Original	-
		0	N ₂	35.3	890	Sodium +2% O ₂ reaction	B
		7.1 x 10 ⁻⁷	N ₂ + fuel†	37.4	921	DBA fuel vapor venting	D
		4.5 x 10 ⁻³	N ₂ + fuel†	27.8	807	Venting to equip cell and cavity	F
		24.5	N ₂ + fuel†	11.9	81	Heat transfer to wall	-
10	Alt Hot Cell	0	Air	14.7	80	Original	-
		0	0.52 N ₂	107.5	1930	Sodium air reaction	B
		4.72 x 10 ⁻⁷	0.48 Na(g)	-	-	-	-
		4.72 x 10 ⁻⁷	0.52 N ₂ 0.48 Na(g) + fuel	109	1955	DBA fuel vapor venting	D
		3.2 x 10 ⁻³	0.52 N ₂ 0.48 Na(g) + fuel†	68.5	1644	Venting to equip cell and cavity	F
		24	0.52 N ₂ 0.48 Na(g) + fuel†	17.5	82	Heat transfer to walls	-
11	Alt Hot Cell	0	Inert	14.7	80	Original	-
		0	N ₂	33.6	812	Sodium +2% O ₂ reaction	B
		7.25 x 10 ⁻⁷	N ₂ + fuel	35.8	966	DBA fuel venting	D
		3.64 x 10 ⁻³	N ₂ + fuel	24.1	720	Venting to equip cell and cavity	F
		13.13	N ₂ + fuel	11.0	80	Heat transfer to walls	-
12	Equip, Cells, and Cavity	0	Inert	14.7	100	Original	-
		0	N ₂	47.5	1290	2% O ₂ reaction	F
		3.26 x 10 ⁻³	N ₂ + Na(g)	95.5	1704	Vent from rect hot cell-air	-
		11.36	N ₂ + Na(g)	23.5	80	Heat transfer to walls	-
13	Equip, Cells, and Cavity	0	Inert	14.7	100	Original	-
		4.5 x 10 ⁻³	Inert	27.8	290	Vent from rect hot cell-inert	F
		2	Inert	20	30	Heat transfer to walls	-
14	Equip, Cells, and Cavity	0	Inert	14.7	100	Original	-
		0	N ₂	35.8	663	2% O ₂ reacting with Na(g)	F
		3.2 x 10 ⁻³	N ₂ + Na(g)	68.5	1018	Vent from alt hot cell-air	-
		16.9	N ₂ + Na(g)	25	80	Heat transfer to walls	-
15	Equip, Cells, and Cavity	0	Inert	14.7	100	Original	-
		3.64 x 10 ⁻³	Inert	24.1	235	Vent from alt hot cell-inert	F
		5.0	Inert	18.5	80	Heat transfer to walls	-

*Weight fraction

†Fuel vapor (negligible weight fraction compared to other gas constituents)

§Condensation during cooling neglected

() Values in parentheses are for 1200°F sodium

Table 4. Summary of Results Under DBA Venting Conditions

4. Design Basis Accident, Venting to Hot Cell

The results of venting of DBA-vaporized fuel from the reactor vessel to the hot cell, after the reaction of 20-tons of expelled sodium with the oxygen in the cell, calculated according to the method given in Section IV-C, are shown in Table 4 (Cases 1 through 4). The initial conditions of the fuel vapor in the reactor vessel after explosive disassembly, but prior to venting to the hot cell, were as follows:

Fuel vapor mass = 800 lb (given in Section III),

Fuel vapor volume = 340 ft³*

Pressure = 60 atm*, and

Temperature = 9450°R*.

In Cases 1 and 3, the pressure in the hot cell, after cooling to the proximity of the initial temperature, is higher than atmospheric. This results from neglecting the condensation of the sodium vapor during the cooling period.

5. DBA Venting to Reactor Vessel Cavity

The results for Accident Condition E, fuel vapor venting to the reactor vessel cavity (without venting to the hot cell), are shown in Table 4 (Case 5).

6. DBA Venting to Equipment Cells and Reactor Cavity

The venting of the pressure in the hot cell, after the DBA (Accident Condition D), to the primary system equipment cells and reactor vessel cavity (Accident Condition F) was computed as in the previous cases of venting to the hot cell and the reactor cavity alone. A typical set of results obtained from the Pressure Equilibration Code[†] is presented in Figure 14 which shows gas pressure, temperature, and mass in the rectangular hot cell and in the equipment cell as a function of time during venting. The results for Accident Condition F are shown in Table 4 (Cases 8-15). Cases 8-11 (Table 4) yield the same information as that in Cases 1-4, with the exception of including venting to the equipment cells and reactor cavity before allowing heat transfer to the hot cell walls to take place. Cases 12-15 give the pressure and temperature in the reactor

*Computed from Equation of State in APDA-119.

† PEQUIB I

Figure 14. Typical Results, PEQUIB I Code (Rectangular Hot Cell, Vented to Equipment Cell and Reactor Cavity, Accident Condition F)

cavity and the equipment cell, after venting and subsequent heat transfer to the walls in these volumes.

In Cases where there was venting from the hot cell to the equipment cell (Cases 8-15) the calculations proceeded as follows. After the pressure and temperature in the hot cell were established from the sodium-air reaction, a certain amount of gas was allowed to vent into the equipment cell and react with the 2% oxygen there. This raised the pressure and temperature in the hot cell. By use of the PEQUIB I Code (Section IV-C) the equilibrium pressure and the corresponding temperature in the hot cell and equipment cell respectively, were calculated. From this point, the temperature and pressure in each cell were calculated by use of the TAP code with no allowance for pressure equilibration between the two cells during cooling. For this reason, the pressure in the hot cell at the end of the cooling period is slightly different than the pressure in the equipment cells. It should be noted that the time scale for venting is shorter by a few orders of magnitude than the time scale for heat transfer; therefore, neglect of heat transfer effects during venting is justified.

Comparison of Cases 1 and 3 with Cases 8 and 10, respectively, (Table 4) shows that venting to the equipment cells reduces the maximum pressure in the rectangular hot cell from 130 to 95 psia and in the alternate hot cell from 109 to 60 psia. By contrast, the maximum pressure for the inerted cell without venting is 35.8 and 44.5 psia for the rectangular and cylindrical hot cells, respectively.

7. Decay of Gas Temperature and Pressure

The decay of gas temperature and pressure in the hot cell and venting volume after the various accidents (except the pool fires) was calculated by use of the TAP code, see Section IV-D. Typical decay curves for various accident conditions are shown in Figures 15 through 18. As can be seen from these figures, most of the cooling occurs in a few hours. Because of an average wall thickness being used in these calculations, it is of interest to examine the effect of wall thickness on the pressure and temperature decay curves. Figure 15 shows curves for wall thicknesses of 4.2 and 5.2 ft;* as indicated, the effect is negligible. This can be attributed to the fact that the heat content in the gaseous mixture is small compared to that of the containment wall heat sink.

*The curves in Figure 15 are for a wall thickness of 4.2 ft; the circle symbols plotted are the results for a 5.2 ft case.

Figure 15. Gas Temperature and Pressure History After Accident Condition D, Rectangular Hot Cell, Air

Figure 16. Gas Temperature and Pressure History After Accident Condition D, Rectangular Hot Cell, Inert

Figure 17. Gas Temperature and Pressure History in Rectangular Hot Cell After Accident Condition D, Air, Venting to Equipment Cells

Figure 18. Gas Temperature and Pressure History in Equipment Cells After Venting From Rectangular Hot Cell, Air, Accident D

Figure 19. Rectangular Hot Cell Wall Node Temperature History After Accident Condition D, Air

Figure 20. Cylindrical Hot Cell Wall Node Temperature History After Accident Condition D, Air

Figures 19 and 20 show the wall temperature history during the decay period calculated from the TAP code for the maximum accident conditions studied. The large heat capacity of the concrete hot cell walls keeps the wall temperatures low.

8. Leakage of Outer Containment

The results of calculations made with the CELLEAK, see Section IV-F, code to determine the pressure and temperature history in the outer containment due to leak rates of 5, 20, and 100%/day from the hot cell, after Accident Conditions C, D, and F, are shown in Table 5. Typical curves of results obtained by use of CELLEAK are shown in Figure 21. The results in Table 5 indicate that even at the highest leak rate, the pressure buildup in the outer containment is rather small. This is essentially due to the fact that the large pressure reduction in the hot cell occurs rapidly due to temperature decay (via wall heat transfer), rather than by leakage.

9. Effect of Increased Sodium Temperature

Results for several selected cases with an increase in sodium temperature to 1200°F is shown in Table 6. It can be seen from Table 6 that an increased sodium temperature of 1200°F results in less than a 10% increase in the maximum pressure rise for the various accidents in a hot cell with an air atmosphere. The increase in pressure rise for the higher initial sodium temperature for accidents in the inerted hot cell is relatively more important than for air, amounting to about 40%. The effect of increasing the initial sodium temperature is less important in the case of the air-filled cell, since the magnitude of the energy release from the sodium-air reaction is considerably larger than the increase in the energy content of the sodium from 700 to 1200°F.

B. NO-HOT-CELL STUDIES

Results for Accident Conditions H, I, J, and K (without a hot cell) are shown in Table 7. The pressure and temperature history for accident conditions H and J are shown in Figures 22 and 23, respectively. The expulsion of 20 tons of sodium into the outer containment yields maximum pressures which fall at the lower end of the curve shown in Figure 11, namely the lower sodium-oxygen molar ratio regime, due to the large volume of this containment.

TABLE 5
LEAKAGE TO OUTER CONTAINMENT

Accident Condition	Hot Cell	Hot Cell Atmos	Hot Cell Leak Rate (%/d)*	Max Press in Hot cell (psia)	Max Press in Outer Cont, P ₁ max (psia)	Mass Fraction Leaked	Time to P ₁ max (hr)
C Nozzle sodium spray fire	Rect	Air	5	47.7	14.77	1.0×10^{-2}	32.9
		Air	20	47.7	14.8	2.27×10^{-2}	12.9
		Air	100	47.7	14.97	4.66×10^{-2}	3.25
	Alt	Air	5	59.8	14.76	1.72×10^{-2}	51.5
		Air	20	59.8	14.79	3.17×10^{-2}	16.3
		Air	100	59.8	14.87	7.26×10^{-2}	5.9
D Sodium expulsion and DBA	Rect	Air	5	128.6	15.4	1.35×10^{-1}	133
		Air	20	128.6	16.1	2.98×10^{-1}	95
		Air	100	128.6	16.3	3.22×10^{-1}	18.6
		Inert	5	37.1	14.7	7.84×10^{-4}	2.58
		Inert	20	37.1	14.7	2.72×10^{-3}	1.98
		Inert	100	37.1	14.7	9.25×10^{-3}	0.78
	Alt	Air	5	109.1	15.4	2.90×10^{-1}	358
		Air	20	109.1	15.6	3.44×10^{-1}	115.2
		Air	100	109.1	15.7	3.64×10^{-1}	24.6
		Inert	5	35.7	14.7	6.68×10^{-4}	2.24
		Inert	20	35.7	14.7	2.35×10^{-3}	1.80
		Inert	100	35.7	14.7	8.38×10^{-3}	0.80
E Item D vent to equipment cells+ reactor cavity	Rect	Air	5	94.6	15.51	1.35×10^{-1}	212
		Air	20	94.6	15.7	1.70×10^{-1}	69.4
		Air	100	94.6	15.87	1.82×10^{-1}	12.3
	Alt	Air	5	68.3	15.12	8.73×10^{-2}	154
		Air	20	68.3	15.20	1.22×10^{-1}	59.0
		Air	100	68.3	15.25	1.38×10^{-1}	13.1

*Leakage at a design pressure of 15 psig.

TABLE 6
EFFECT OF INCREASED SODIUM TEMPERATURE ON PEAK PRESSURE
FOR SEVERAL ACCIDENT CONDITIONS

Accident Condition	Cell	Cell Atmos	Peak Pressure 700°F Sodium (psig)	Peak Pressure 1200°F Sodium (psig)	Condition
A	Rect	Air	26.8	27.88	10-ton Na spill, pool fires
A	Rect	2% N ₂	4.3	7.2	10-ton Na spill, pool fires
B	Rect	Air	111	123	20-ton Na expulsion
B	Rect	2% N ₂	20.6	29.6	20-ton Na expulsion
D	Rect	Air	112	124	20-ton Na expulsion followed by DBA fuel vapor venting into hot cell
D	Rect	2% O ₂	22.7	31.8	20-ton Na expulsion followed by DBA fuel vapor venting into hot cell
D	Cyl	2% O ₂	21.1	31.1	20-ton Na expulsion followed by DBA fuel vapor venting into hot cell
E	Reactor Cavity	2% O ₂	29.8	43.3	20-ton Na expulsion followed by DBA fuel vapor venting into lower reactor cavity

TABLE 7
SUMMARY OF ACCIDENT RESULTS WHEN HOT CELL IS EXCLUDED

Accident Condition	Time (hr)	Outer Containment Atmosphere (lb)	Pressure (psia)	Temperature (°F)	Change of Conditions
H	0	Air = 18.9×10^4	14.7	80	Reaction of 20 tons of DBA expelled sodium (700°F) with air
	0	N ₂ = 14.3×10^4 O ₂ = 3×10^4 Na ₂ O(S) = 5.4×10^4 Na(g) = 0.061×10^4 NaO(g) = 0.088×10^4	82	2710	
	25	Same as above, no condensation allowed	14.3	93	
I	0	Air	14.7	80	20 ton spill of 700°F sodium (pool fire)
	0.21	(~17% O ₂)	42.5	1190	Peak pressure
J	0	Air = 18.9×10^4	14.7	80	Peak pressure 1000 lb/min nozzle spray (for 10 min) and simultaneous heat transfer to the walls
	0.167	Air	36.8	900	
	30		14.7	80	
K			No significant differences in results from Item H.		DBA fuel vapor venting following Item H sodium expulsion

Figure 21. Typical CELLLEAK Code Results After Accident Condition D, Rectangular Hot Cell – Air, 20% per Day

Figure 22. Gas Pressure and Temperature History, Outer Containment, After Accident Condition H

Figure 23. Gas Pressure and Temperature History, Outer Containment, Accident Condition J

C. VALIDITY OF CALCULATIONS AND AREAS OF UNCERTAINTIES

The theoretical calculations show that the maximum pressure generated in the cell would correspond to the case in which the sodium is homogeneously and instantaneously dispersed in the air-filled cell. The lower limit for pressure generation corresponds to the case in which the sodium burns as a pool.

In reality, it can be expected that neither of these limits will be attained and that the maximum cell pressure rise will fall somewhere in between; a finite time is required for dispersal and breakup of the liquid into small particles.

The time needed to break up a liquid jet from a nozzle into small droplets is approximately given by the equation, Reference 4,

$$\tau = \sqrt{\frac{\rho_l}{\rho_{air}}} \left(\frac{a}{u} \right),$$

where

a = nozzle radii,

ρ = density, and

u = jet velocity.

By taking the velocity of the slug as 160 ft/sec and its diameter as 16 ft, the time for breakup is found to be

$$\tau = \sqrt{\frac{50}{(7.35 \times 10^{-2})}} \left(\frac{8}{160} \right) \approx 1.3 \text{ sec}.$$

By assuming that the same velocity exists through the flight, the total time to transverse the 176 ft needed for the slug to fall on the floor intact (88 ft hot cell height) is 1.35 sec. This highly simplified model appears to indicate that it is unrealistic to expect a complete dispersal of the sodium slug into small liquid particles.

Surface burning, deflection from the wall, and neglect of the presence of the lifted plug are all factors which would further promote dispersal. On the other hand, the finite time required for combustion of liquid droplets would prevent portions of them from being completely burned before dropping to the floor.

In the light of the large uncertainty of the amount of sodium dispersal, the accuracy of the limit calculations (pool, complete dispersal) is not deemed to be important. Experiments performed by Humphreys⁽⁵⁾ for sodium/oxygen molar ratios up to 4:1 indicate that, under certain conditions, the theoretical upper limit pressures may be reached; however, his experiments were conducted in a scaled model, and since scaling laws are not available, it remains to be shown that the results are applicable to large containment volumes.

VI. CONCLUSIONS

The maximum pressure rises generated in the FFTF hot cells for the range of accident conditions and hot cell atmospheres studied are estimated to vary from 3 to 112 psig for an initial sodium temperature of 700°F, as summarized in Table 8 below.

TABLE 8
MAXIMUM PRESSURE-RISE COMPARISON OF
HOT CELLS AND ATMOSPHERES
(psig)

Cell Atmosphere	DBA Sodium and Fuel Expulsion		Nozzle Spray Fire		Pool Fire	
	Rectangle	Cylinder	Rectangle	Cylinder	Rectangle	Cylinder
Air	112	94	44	42	27	22
Inert	23	21	--	--	4	3

The results of selected cases at an initial sodium temperature of 1200°F yield higher pressure rises (7 to 124 psig) than those for the 700°F cases in the rectangular hot cell. For any given accident, the pressure generated in the rectangular hot cell is higher than that in the cylindrical hot cell. In the case of the most severe accident condition (the expulsion of 20 tons of sodium into the air-filled hot cell), the smaller volume of the cylindrical cell represents a sodium-oxygen molar ratio which is higher than the ratio where the maximum theoretical pressure occurs; i.e. ~7:1, see Figure 11. A reduction in the assumed quantity of sodium expelled by the DBA in the molar ratio range of interest to the present study would not lead to proportionately lower maximum pressures. For example in the case of the rectangular cell, lowering the expelled quantity of sodium by a factor of 4 (to 5 tons) results in a reduction of only ~33% in the theoretical pressure. A similar reduction in the quantity of sodium in the cylindrical cell produces even less of a reduction in the theoretical pressure.

The assumption that a large quantity of DBA-expelled sodium disperses in sufficiently fine particles so as to react instantaneously and in equilibrium with all of the available oxygen in the hot cell is difficult to justify; hence, the maximum pressure estimated is very conservative. One would anticipate that the maximum pressure will probably be a value between that for the pool fire and that for the sodium expulsion cases.

For the specified quantity of fuel vaporized in the DBA; namely, 800 lb, the contribution of the fuel energy is small compared with the energy released from sodium-air reaction; hence, venting of the fuel vapor into the hot cell after the expulsion of the sodium does not result in a significant increase in the pressure due to the chemical reaction.

The mitigative effectiveness of the use of an inert atmosphere in the hot cell is clearly demonstrated. The use of adjacent venting volumes to reduce the pressure in the hot cell during the DBA appears to be worthwhile; however, the venting area (5 ft^2) specified for the study appears to be insufficient, since the time for equilibration, ~ 10 seconds, is too slow to effect the desired pressure reduction.

The pressure buildup in the outer containment due to leakage from the hot cell is relatively small, amounting to less than 2 psig for the worst hot cell accident.

The maximum pressures in the outer containment, in the absence of the hot cell, for the equivalent accidents, range from 22 to 67 psig. The maximum theoretical pressure in the outer containment for the 20-ton sodium expulsion is substantially lower than that in the hot cell due to the lower sodium-oxygen molar ratio, see Figure 11. One obvious advantage of the use of the hot cell is that it would greatly reduce the design pressure requirements for the outer containment.

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APPENDIX A

DESCRIPTION OF SOFIRE I MODEL

The basic equations used in the SOFIRE I Code are described below.

1. Heat balance on flame

a. Convection heat transfer from the flame to V1 gas, QFG

$$QFG = HFG(TF - T1) + C_s(EPFG)(TF^4 - T1^4)$$

b. Conduction heat transfer from the flame to sodium pool, KFS

$$KFS = C_1 + C_2(TF + TS) - C_3(TF + TS)^2$$

c. Convection heat transfer from the flame to sodium pool, QFS

$$QFS = \left(\frac{KFS(R)}{[C_4(TS + TF)]^{1.5}CS} + HFS \right) (TF - TS) + C_5EPFS(TF^4 - TS^4)$$

d. The ith step flame temperature is calculated by

$$TF = TF_{(i-1)} - [QFG + QFS - HC(R)] / \left[\frac{KFS(R)}{C_4(TS_{(i-1)} - TF)^{1.5}CS} + HFS + HFG + 4[C_5(EPFS) + C_5(EPFG)(TF_{(i-1)})^3] \right] \quad \dots (A-1)$$

2. Heat balance on F1 and V2 gas

a. Convection heat transfer from V1 gas to cell wall, Q1

$$Q1 = H1(T1 - TW1) + C_sEP1(T1^4 - TW1^4)$$

b. Convection heat transfer from V1 gas to cell cooling system, Q6

$$Q6 = Q60 + Q61(T1 - T0)$$

c. Convection heat transfer from V2 gas to thick room wall, Q2

$$Q2 = H2(T2 - TW3) + C_5EP2(T2^4 - TW3^4)$$

d. Convection heat transfer from V2 gas to heat absorbing masses, Q3

$$Q3 = H3(T2 - T3) + C_5EP3(T2^4 - T3^4)$$

e. Convective heat transfer from V2 gas to thin room wall, Q5

$$Q5 = H5(T2 - T5) + C_5EP5(T2^4 - T5^4)$$

f. Convective heat transfer from V2 gas to room cooling system, Q7

$$Q7 = Q70 + Q71(T2 - T0)$$

g. The ith step cell gas temperature is calculated by

$$T1 = T1_{i-1} + \left[(QFG)(A0) - (Q1)(A1) - Q6 - (\rho2)(F2)(CV)(T1 - T2) \right. \\ \left. - (\rho0)(CV)(F5)(T1 - T0) - (C_6)(P1)(F1 - F2 - F5) \right] \left[\frac{\Delta t}{(V1)(CV)(\rho1)} \right] \\ \dots (A-2)$$

h. The ith step room gas temperature is calculated by

$$T2 = T2_{i-1} + \left[(\rho1)(F1)(CV)(T1 - T2) + \left(\frac{\rho0}{CV} \right) (F3)(T0 - T2) - Q2(A2) \right. \\ \left. - (Q3)(A3) - (Q5)(A5) - Q7 + (C6)(P)(F1 - F2 - F4 + F3) \right] \left[\frac{\Delta t}{(V2)(CV)\rho2} \right] \\ \dots (A-3)$$

i. The ith step cell wall temperature is calculated by

(inner-wall slab)

$$TW1 = TW1_{i-1} + \left[\frac{(\Delta t)(KC)}{(\rho C)(CpC)} \right] \left[\frac{(Q1)}{(KC)(X1)} - \frac{(TW1 - TW2)}{(X1)(X1 + X2/2)} \right] \dots (A-4)$$

(center-wall slab)

$$TW2 = TW2_{i-1} + \left[\frac{(\Delta t)(KC)(TW1 + T0 - 2TW2)}{(X2)(X1 + X2/2)(\rho C)(CpC)} \right] \dots (A-5)$$

- j. The ith step room wall and heat absorbing mass temperatures are calculated by

(inner-wall slab)

$$TW3 = TW3_{i-1} + \left[\frac{(\Delta t)(2)}{(\rho W)(C_p W)(X3)} \right] \left[Q2 - \frac{(KW)(TW3 - TW4)}{X3} \right] \dots (A-6)$$

(center-wall-slab)

$$TW4 = TW4_{i-1} + \left[\frac{(\Delta t)(2)}{(\rho W)(C_p W)(X3)} \right] \left[\frac{KW(TW3 - TW4)}{X3} - HW(TW4 - T0) - C_5(EPW)(TW4^4 - T0^4) \right] \dots (A-7)$$

$$T3 = T3_{i-1} + \frac{(\Delta t)(Q3)(A3)}{(M3)(C_p 3)} \dots (A-8)$$

$$T5 = T5_{i-1} + \left[\frac{(\Delta t)}{(\rho 5)(C_p 5)(X5)} \right] \left[Q5 - HW(T5 - T0) - C_5(EPW)(T5^4 - T0^4) \right] \dots (A-9)$$

3. Heat Balance on Sodium Pool

(upper pool slab)

$$TS1 = TS1_{i-1} + \left[\frac{(2)(\Delta t)}{(\rho S)(ZS)(C_p S)} \right] \left[QFS + \frac{QDO}{2} - (C_7)(HC)(R) - (KS) \frac{(TS1 - TS2)}{ZS} \right] \dots (A-10)$$

(lower pool slab)

$$TS2 = TS2_{i-1} + \left[\frac{(2)(\Delta t)}{(\rho S)(ZS)(C_p S)} \right] \left[\frac{QDO}{2} + \frac{KS(TS1 - TS2)}{ZS} - \frac{2(TS2 - TC1)}{KC/Z1} \right] \dots (A-11)$$

(upper floor slab)

$$TC1 = TC1_{i-1} + \left[\frac{(\Delta t)(KC)}{(\rho C)(CpC)} \right] \left[\frac{(2)(TS2)}{Z1^2} + \frac{(2)(TC2)}{(Z1)(Z1+Z2)} - \left(\frac{Z1+Z2}{Z1} \right) (TC1) \right] \dots (A-12)$$

(middle floor slab)

$$TC2 = TC2_{i-1} + \left[\frac{(\Delta t)(KC)}{(\rho C)(CpC)} \right] \left[\frac{(2)(TC1)}{Z2(Z1+Z2)} + \frac{(2)(TC3)}{Z2(Z2+Z3)} - \left(\frac{Z2+Z3}{Z1+Z2} \right) (TC2) \right] \dots (A-13)$$

(lower floor slab)

$$TC3 = TC3_{i-1} + \left[\frac{(\Delta t)(KC)}{(\rho C)(CpC)} \right] \left[\frac{(2)(TC2)}{Z3(Z2+Z3)} + \frac{(2)(TC3)}{Z3^2} - \left(\frac{2}{Z3(Z2+Z3)} + \frac{2}{Z3^2} \right) (TC3) \right] \dots (A-14)$$

4. Mass Balance on V1 and V2 gas

a. Cell ventilation term F5

$$F5 = F50 + F51(P0 - P)$$

b. Room ventilation term, F3 and F4

$$\text{(inlet)} \quad F3 = F41(P0 - P) + 10(F42) \sqrt{P0 - P}$$

$$\text{exhaust} \quad F4 = F40$$

c. Counter flow term F1 and F2

$$\text{(upward)} \quad F1 = \left(\frac{AH}{2} \right) (C_8) \sqrt{(ZC)(\rho_2 - \rho_1)/\rho_1} \dots (A-15)$$

$$\begin{aligned}
(\text{downward}) \quad F2 = F1 &+ \left[\frac{(-QFG)(A0)}{(V1)(CV)} + \frac{(Q1)(A1)}{(V1)(CV)} + \frac{(Q6)}{(V1)(CV)} - \frac{(Q2)(A2)}{(V2)(CV)} \right. \\
&- \frac{(Q3)(A3)}{(V2)(CV)} - \frac{(Q5)(A5)}{(V2)(CV)} - \frac{(Q7)}{(V2)(CV)} + C_9(R)(T1) \\
&- \frac{(F4)(C_6)[P + (T1)(\rho1)/V2]}{(V2)(CV)} + F3 \left[\frac{(\rho0)(T0)}{V2} + \frac{(C_6)P}{(V2)(CV)} \right] \\
&- (F5) \left[\frac{(\rho0)(T0)}{V1} + \frac{(C_6)(P)}{(V1)(CV)} \right] \Bigg/ \left[(\rho1)(T1) \left(\frac{1}{V1} + \frac{1}{V2} \right) \right. \\
&\left. + P \left(\frac{1}{V1} + \frac{1}{V2} \right) \frac{C_6}{CV} \right] \quad \dots (A-16)
\end{aligned}$$

5. Density of cell gas (due to oxygen depletion F1 and F5)

$$\rho1 = \rho1_{i-1} + \left[(-F1)\rho1 + (F2)(\rho2) + (F5)(\rho0) - (C_9)(A0)(R) \right] \left[\frac{\Delta t}{V1} \right] \quad \dots (A-17)$$

6. Density of room gas (due to F2, F3, and F4)

$$\rho2 = \rho2_{i-1} + \left[\left((F1)(\rho1) + (F2)(\rho2) \right) - (F4)(\rho2) + (F3)(\rho0) \right] \left[\frac{\Delta t}{V2} \right] \quad \dots (A-18)$$

7. System pressure

$$P = \frac{(P0)(T1)(\rho1)}{(T0)(\rho0)} \quad \dots (A-19)$$

8. Sodium burning rate

$$R = (C_{10}) \left\{ C1_{i-1} + \left[\left(-(F1)(C1) + F2(C2) \right) + (F5)(C5) - (C_9)(A0) \frac{(R)(\Delta t)}{V1} \right] \right\} \quad \dots (A-20)$$

LIST OF CONSTANTS

C_1	2.3×10^{-3}
C_2	1.325×10^{-5}
C_3	9.675×10^{-10}
C_4	1.73×10^{-5}
CS	Concentration of sodium vapors above flame
C_5	1.74×10^{-9}
C_6	1.285×10^{-3}
C_7	0.318
C_8	2.89×10^4
C_9	0.348
C_{10}	6.51×10^2

The terms are defined on the following pages.

SOFIRE NOMENCLATURE LIST

A0	Fire Surface Area	ft ²
A1	Cell Wall Area	ft ²
A2	Room Wall No. 2 Area	ft ²
A3	Heat Absorbing Area	ft ²
A5	Room Thin Wall Area	ft ²
AH	Area of Cell Opening	ft ²
C0	O ₂ Concentration in Air	lb/ft ³
C1	O ₂ Concentration in Cell	lb/ft ³
C2	O ₂ Concentration in Room	lb/ft ³
CpC	Specific Heat of Concrete	Btu/lb °F
CpS	Specific Heat of Sodium	Btu/lb °F
CpW	Specific Heat of Wall 2	Btu/lb °F
Cp3	Specific Heat of Wall 3	Btu/lb °F
Cp5	Specific Heat of Wall 5	Btu/lb °F
CV	Specific Heat of Na Vapor	Btu/lb °F
HFS	Heat Transfer Coefficient Flame to Na	Btu/hr-ft ² °F
HFG	Heat Transfer Coefficient Flame to Gas	Btu/hr-ft ² °F
HW	Heat Transfer Coefficient Wall to Environment	Btu/hr-ft ² °F
H1	Heat Transfer Coefficient Gas to Wall 1	Btu/hr-ft ² °F
H2	Heat Transfer Coefficient Gas to Wall 2	Btu/hr-ft ² °F
H3	Heat Transfer Coefficient Gas to Wall 3	Btu/hr-ft ² °F
H5	Heat Transfer Coefficient Gas to Wall 5	Btu/hr-ft ² °F
HC	Na Heat of Combustion	Btu/lb
KC	Conductivity of Concrete	Btu/hr-ft ² °F

KW	Conductivity of Wall 2	Btu/hr-ft ² °F
M3	Mass of Heat Absorber	lb
QDO	Decay Heat in Na Pool	Btu/hr-ft ²
Q60	Cell Cooler Constant	Btu/hr
Q61	Cell Cooler Constant	Btu/hr
Q70	Room Cooler Constant	Btu/hr
Q71	Room Cooler Constant	Btu/hr'
ΔT	Minimum Calculation Time Step	hr
ΔT Max	Maximum Calculation Time Step	hr
TMAX	Maximum Fire Limit	hr
T0	Temperature Cell Gas	°R
TC1	Temperature Cell Floor Slab 1	°R
TC2	Temperature Cell Floor Slab 2	°R
TC3	Temperature Cell Floor Slab 3	°R
TF	Flame Temperature	°R
TS1	Na Upper Surface Temperature	°R
TS2	Na Lower Surface Temperature	°R
TW1	Temperature of Wall 1	°R
TW2	Temperature of Wall 2	°R
TW3	Temperature of Wall 3	°R
TW4	Temperature of Wall 4	°R
T1	Temperature of Cell Gas	°R
T2	Temperature of Room Gas	°R
T3	Temperature of Heat Abs Mass	°R
T5	Temperature of Wall 5	°R
Tmin	Minimum Fire Temperature	°R

V1	Cell Volume	ft ³
V2	Room Volume	ft ³
X1	Thickness of Cell Wall Slab	ft
X2	Thickness of Cell Wall Slab	ft
X3	Thickness of Room Wall 3	ft
X5	Thickness of Room Wall 5	ft
ZC	Height of Cell	ft
ZS	Depth of Na Pool	ft
Z1	Cell Floor Slab Thickness	ft
Z2	Cell Floor Slab Thickness	ft
Z3	Cell Floor Slab Thickness	ft
$\Delta 0$	Heat Balance Error Limit	
EPFG	Emissivity Flame to Gas	Btu/ft ² -hr
EPFS	Emissivity Flame to Na	Btu/ft ² -hr
EPW	Emissivity Wall to Environment	Btu/ft ² -hr
EP1	Emissivity Gas to Wall 1	Btu/ft ² -hr
EP2	Emissivity Gas to Wall 2	Btu/ft ² -hr
EP3	Emissivity Gas to Wall 3	Btu/ft ² -hr
EP5	Emissivity Gas to Wall 5	Btu/ft ² -hr
ρC	Density of Concrete	lb/ft ³
ρNa	Density of Na	lb/ft ³
ρW	Density of Cell Wall	lb/ft ³
$\rho 0$	Density of Air	lb/ft ³
$\rho 5$	Density of Wall 5	lb/ft ³
N1	CRT Print Step 1	hr

N2	CRT Print Step 2	hr
N3	CRT Print Step 3	hr
PT2	Print Limit	hr
PT3	Print Limit	hr
C5	O ₂ Concentration of Cell Inlet Gas	lb/ft ³
F40	Room Gas Flow Constant	ft ³ /hr
F41	Room Gas Flow Constant	ft ³ /hr
F42	Room Gas Flow Constant	ft ³ /hr
F50	Cell Gas Flow Constant	ft ³ /hr
F51	Cell Gas Flow Constant	ft ³ /hr
P	Initial Pressure	psf
ρ_1	Density of Cell Gas	lb/ft ³
ρ_2	Density of Room Gas	lb/ft ³
AK25	Constant = 1.0	
AK51	Constant to Locate Heat Absorbing Mass in Cell (AK51 = 1.0) or Secondary (AK51 = 2.0)	

APPENDIX B

ADIABATIC EQUILIBRIUM SODIUM-AIR REACTION

From thermodynamic considerations, the condition for chemical equilibrium is attained when the total free energy of the various species is minimum. If f_i^g and f_h^c denote the free energy of a specie i and of h , in a gaseous and condensed phase respectively, the total free energy of the mixture is,

$$F = \sum_i^n f_i^g + \sum_i^n f_h^c \quad \dots(B-1)$$

For a constant value process, the free energy of a gaseous specie is

$$f_i^g = \left\{ X_i^g \left(\frac{F^\circ - H_{298}^\circ}{RT} + \frac{\Delta H_{f,298}^\circ}{RT} \right)_i + \ln \left[\frac{\left(\sum_i^n X_i^g \right) RT}{V} \right] - 1 + \ln \left[\frac{X_i^g}{\sum_i^n X_i^g} \right] \right\} \dots(B-2)$$

The free energy of a condensed specie is

$$f_h^c = X_h^c \left[\left(\frac{F^\circ - H_{298}^\circ}{RT} \right)_h + \left(\frac{\Delta H_{f,298}^\circ}{RT} \right)_h \right] \quad \dots(B-3)$$

Combining Equations B-1 through B-3, the expression for the total free energy of the mixture becomes

$$F(X_i) = \sum_i^n \left\{ X_i^g \left[\frac{(F^\circ - H_{298}^\circ)}{RT} + \frac{\Delta H_{f,298}^\circ}{RT} \right]_i + \ln \frac{\left(\sum_i^n X_i^g \right) RT}{V} \right. \\ \left. - 1 + \ln \frac{X_i^g}{\sum_i^{n-1} X_i^g} + \sum_h^p X_h^c \left[\left(\frac{F^\circ - H_{298}^\circ}{RT} \right)_h + \left(\frac{\Delta H_{f,298}^\circ}{RT} \right)_h \right] \right\} \quad \dots(B-4)$$

It is now required to find the composition of the mixture X_i and X_h which will minimize Equation B-4 and at the same time satisfy the mass and energy balance requirements.

1. Mass Balance

If a_{iJ}^g and a_{hJ}^c are the number of atoms of the J^{th} element in the i^{th} gaseous specie and of the J^{th} element in the h^{th} condensed specie respectively, the mass balance requires that

$$\sum_i^n a_{iJ}^g X_i^g + \sum_h^p a_{hJ}^c X_h^c = b_J, \quad (J = 1, 2, \dots, m); \quad \dots(B-5)$$

where m is the total number of reactants in the system.

2. Energy Balance

From heat balance considerations, the chemical heat of the reaction plus the sensible heat of the reactants in the absence of any heat losses, equals the sensible heat which is required to raise the products of the reaction to the final system temperature;

$$\sum_i^{h+p} X_i [E_T - E_{298}]_i = \sum_{J=1}^m (X_{\text{re}})_J [E_{T'_J} - E_{298}] + \sum_i^{h+p} X_i \Delta E_{298}, \quad \dots(B-6)$$

where

$(X_{\text{re}})_J$ = initial concentration of the J^{th} reactant,

T'_J = initial temperature of the J reactant,

E_T, E_{298} = energy at the final system temperature and at 298°K respectively,

ΔE_{298} = energy of reaction at 298°K ,

h = total number of gaseous species, and

p = total number of condensed species.

Equations B-4, B-5, and B-6 are subject to the requirements that $F(X_i)$ be a minimum. These equations were programmed by ANL for solution on a digital computer and referred to as the Chemical Equilibrium Calculations Program (see References 6 and 7).

ADIABATIC SODIUM, OXYGEN REACTION FOR LOW OXYGEN CONTENT

A simplification of the method described in Appendix B was used for calculations involving expulsion of sodium into the hot cell with an inert atmosphere (2 v/o oxygen) or release of sodium into the inerted venting volumes (lower reactor cavity and primary equipment cells). For the reaction of sodium with 2 v/o oxygen, complete consumption of the oxygen is assumed due to the large amount of excess sodium present. In addition, since equilibrium temperatures will be considerably lower than for the sodium-air reaction for the sodium temperatures in this study, the only reaction product which is formed is Na_2O ; e. g., the reaction $\text{Na}_2\text{O} \rightleftharpoons \text{Na} + \text{NaO}$ does not occur. It is then sufficient to only solve Equations B-5 and B-6 in Appendix B. Equation B-6 then gives:

$$\begin{aligned} & (\text{XC}_p)_{\text{Na}(\ell)\text{ excess}}[T - T_o] + (\text{XC}_p)_{\text{Na}_2\text{O}(\text{c})}[T - T_o] \\ & + (\text{XC}_v)_{\text{N}_2}[T - T_o] = (\text{X}_0\text{C}_p)_{\text{Na}(\ell)}[T_{\text{Na}(\ell)} - T_o] + (\text{X}\Delta\text{H}_{\text{f},\text{o}})_{\text{Na,reacted}}, \dots(\text{B-7}) \end{aligned}$$

where subscript 0 designates (a) reference temperature, which is also the initial temperature of the N_2 and O_2 in the system; and (b) the initial number of moles.

From a mass balance:

$$\left. \begin{aligned} \text{X}_{\text{Na}(\ell)\text{ reacted}} &= 2\text{X}_{\text{Na}_2\text{O}(\text{c})}, \\ \text{X}_{\text{Na}(\ell)\text{ excess}} + \text{X}_{\text{Na}(\ell)\text{ reacted}} &= \text{X}_{0,\text{Na}(\ell)}, \text{ and} \\ (1/4)\text{X}_{\text{Na}(\ell)\text{ reacted}} &= \text{X}_{0,\text{O}_2(\text{g})}. \end{aligned} \right\} \dots(\text{B-8})$$

Thus,

$$\text{X}_{\text{Na}_2\text{O}(\text{c})} = (1/2)\text{X}_{0,\text{O}_2(\text{g})},$$

$$\text{X}_{\text{Na}(\ell)\text{ excess}} = \text{X}_{0,\text{Na}(\ell)} - \text{X}_{0,\text{O}_2(\text{g})}, \text{ and}$$

$$\text{X}_{\text{Na}(\ell)\text{ reacted}} = \text{X}_{0,\text{O}_2(\text{g})}.$$

Substituting Equation B-8 into Equation B-7 gives the final system temperature:

$$T = \frac{4X_{O_2(g)}\Delta H_{f,o} + (X_{Na(l)}C_{p,Na(l)})[T'_{Na(l)} - T_o]}{[X_{Na(l)} - 4X_{O_2(g)}]C_{p,Na(l)} + 2X_{O_2(g)}C_{p,Na_2O(c)} + X_{N_2}C_{v,N_2}} + T_o$$

...(B-9)

Equation B-9 gives the final system temperature in terms of the initial concentrations of Na(l) and O₂(g) and the initial temperature T'_{Na} of the sodium.

APPENDIX C

FUEL VAPOR VENTING TO HOT CELL AFTER DBA

The schematic for setting up the basic equations is shown in Figure 3. Subscripts 1 and 2 represent the instantaneous pressure, volume, the temperature of the fuel vapor in the reactor, and the gaseous mixture ($\text{PuO}_2 - \text{UO}_2$, O_2 , NaO , N_2 , Na) in the hot cell, respectively. The reactor and the hot cell are connected by an opening with a cross sectional area A . The problem is to determine the instantaneous pressure and temperature in the hot cell.

For a quasi-steady adiabatic nonviscous flow obeying the ideal gas law, the pressure decay in the reactor cell as a function of time and the back pressure in the hot cell is given by

$$\frac{dP_1}{dt} = - \frac{AP_2 \sqrt{\gamma R T_{01}}}{V_1 \left(\frac{\gamma-1}{2}\right)^{0.5}} \left(\frac{P_2}{P_{01}}\right)^{(\gamma-1)/2\gamma} \left(\frac{P_1}{P_2}\right)^{(\gamma-1)/\gamma} \sqrt{\left(\frac{P_1}{P_2}\right)^{(\gamma-1)/\gamma} - 1}, \dots (C-1)$$

for

$$P_1 \leq \frac{P_2}{\left(\frac{2}{\gamma+1}\right)^{\gamma/(\gamma-1)}};$$

and

$$P_1 = \left[\frac{A(\gamma-1)}{2V_1} \left(\frac{\gamma+1}{2}\right)^{-(\gamma+1)/[2(\gamma-1)]} \sqrt{\gamma R T_{01}} t + 1 \right]^{-2\gamma/(\gamma-1)} P_{01}, \dots (C-2)$$

for

$$P_1 \geq \frac{P_2}{\left(\frac{2}{\gamma+1}\right)^{\gamma/(\gamma-1)}}.$$

Here, γ is the specific heat ratio, R is the gas constant, and T_{01} and P_{01} are the temperature and pressure in the reactor at time $t = 0$.

The pressure P , is related to the temperature T , by the adiabatic relation

$$\frac{P_1}{P_{01}} = \left(\frac{T_1}{T_{01}} \right)^{\gamma/(\gamma-1)} \quad \dots(C-3)$$

The mass flow m , into the hot cell is given by

$$m = \frac{AP_1}{\sqrt{RT_1}} \left\{ \frac{2\gamma}{\gamma-1} \left[\left(\frac{P_2}{P_1} \right)^{2/\gamma} - \left(\frac{P_2}{P_1} \right)^{(\gamma+1)/\gamma} \right] \right\}^{0.5}, \quad \dots(C-4)$$

for

$$P_1 \leq \frac{P_2}{\left(\frac{2}{\gamma+1} \right)^{\gamma/(\gamma-1)}};$$

and

$$m = \frac{A\sqrt{\gamma} \left(\frac{2}{\gamma+1} \right)^{(\gamma+1)/[2(\gamma-1)]}}{\sqrt{RT}} P_1, \quad \dots(C-5)$$

for

$$P_1 \geq \frac{P_2}{\left(\frac{2}{\gamma+1} \right)^{\gamma/(\gamma-1)}}.$$

Consistent with the assumption of instantaneous mixing of the fuel vapor with the gas in the hot cell, the temperature T_2 there is

$$T_2 = \frac{m\Delta t C_{v,f} T_1 + \left[W_o + \int_0^{\tau} m dt \right] C_{v,n-1} T_{2,\tau}}{C_{v,f} m\Delta t + \left[W_o + \int_0^{\tau} m dt \right] C_{v,n-1}}. \quad \dots(C-6)$$

The first term in the numerator represents the total heat carried by the fuel vapor in an interval time Δt , and the second term represents the total heat content of the gas mixture in the hot cell.

$$\bar{C}_{v,n} = \frac{m(\Delta t)_n C_{vf} + \left[W_o + \int_0^\tau m dt \right] \bar{C}_{v(n-1)}}{m(\Delta t)_n + \left[W_o + \int_0^\tau m dt \right]}, \quad \dots (C-7)$$

where

$$n = 1,$$

$$\tau = \sum_1 \Delta t, \text{ and}$$

W_o = mass of gas in the hot cell, at $t = 0$.

Finally, the pressure in the hot cell is obtained from the ideal gas law

$$P_2 = \left[\frac{W_o}{M_o} + \frac{\int_0^\tau m dt}{M_f} \right] \frac{R_u T_2}{V_2} \quad \dots (C-8)$$

where

M_o, M_f = molecular weights of gas and fuel respectively, and

R_u = universal gas constant.

Equations C-3 through C-8 were programmed for a digital computer (PEQUIB I)* to give the temperature T_2 , and pressure P_2 , as a function of time. The following constants were used in these calculations:

$$\gamma_f = 1.15; \quad C_{v,f} = 0.0477 \text{ Btu/lb-}^\circ\text{R}.$$

*NR Proprietary Information.