SPENT FUEL SHIPPING CASK
ACCIDENT EVALUATION

S. R. Fields

December 1975

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Operated by Westinghouse Hanford Company
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P.O. Box 1970 Richland, WA 99352

Prepared for the U.S. Energy Research and Development
Administration under Contract No. EY-76-C-14-2170

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ACCIDENT EVALUATION

S. R. Fields

Abstract

Mathematical models have been developed to simulate the dynamic behavior, following a hypothetical accident and fire, of typical casks designed for the rail shipment of spent fuel from nuclear reactors, and to determine the extent of radioactive releases under postulated conditions. The casks modeled were the IF-300, designed by the General Electric Company for the shipment of spent LWR fuel, and a cask designed by the Aerojet Manufacturing Company for the shipment of spent LMFBF fuel.

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ACKNOWLEDGMENT

I would like to acknowledge the assistance of R. E. Keyes in adapting the models to the AMCO cask.

S. R. Fields

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SUMMARY

The objective of this study was to develop a series of models to analyze hypothetical spent fuel shipping cask accidents. Although rigorous standards have been developed by the Nuclear Regulatory Commission (NRC) in connection with licensing spent fuel shipping casks, there is a continuing need to develop analytical tools to study extremely-low-probability incidents with potentially serious consequences. This study is intended to contribute to such a body of knowledge. No accident probabilities have been assigned in this study, but there is no doubt that licensed casks comply with all relevant NRC standards.

The casks studied were the General Electric IF-300, designed for the shipment of spent LWR fuel,⁽¹⁾ and a cask designed by the Aerojet Manufacturing Company (AMCO) for shipment of spent LMFBR fuel.⁽²⁾ A set of five models has been developed for the IF-300, and a similar set of models for the AMCO cask. These models simulate cask behavior during normal operating conditions, and during conditions following an accident and fire. The accident evaluated was strictly a hypothetical one; there is no implication that such an accident has ever occurred or will occur.

It was assumed that damage to the casks in the accident included loss of any solar shield, loss of the water in the outer jacket or neutron shield, and a breach in the cask containment. It was further assumed that the fuel pins did not rupture at impact and, consequently, there was no prompt release of fission gases. This set of assumptions was arbitrarily selected as the initial condition of each cask for the analyses. The assumption of a breach in the cask containment is the most influential and, for the IF-300, it was assumed that this breach was due to damage to a pressure relief valve. This must not be interpreted as an implication that this valve is vulnerable to damage or malfunction. On the contrary, the relief valve is not only a well designed and proven component, but is also extremely well protected in the IF-300 design (see Figures 1 and 2 in the Results and Discussion section).

Although the AMCO cask design does not include a pressure relief valve, the same breach flow areas were assumed for the analysis of its behavior

following the accident. This allowed the calculation of the rate of primary coolant loss from the two different types of casks, and the subsequent hypothetical release of fission products, to be based on identical breach areas.

Two breach sizes or flow areas were assumed for each cask. The smallest flow area assumed was 0.025 in.^2 , a reasonable area for a relief valve not fully reseated. The largest flow area assumed was 0.25 in.^2 , a reasonable area for a relief valve sheared off. Cask behavior was evaluated for each of these flow areas, once with the breach up and again with the breach down.

The sets of models developed in this study were used to predict the nature and timing of the release of fission products from the casks following the hypothetical accident, if the primary coolant containment were breached. The arbitrarily selected breach-causing mechanisms, along with other assumed damage to the casks, has been described in the preceding paragraphs. Results obtained from this preliminary analysis, in terms of some key events and their times of occurrence, are summarized in Table i for the IF-300 and in Table ii for the AMCO cask.

When a fuel pin bursts, fission products are released; therefore the pin burst times presented in Tables i and ii also represent fission product release times. The results of Table i show that all of the pins burst in the IF-300. This is equivalent to the release of 11,900 curies of fission gases, about 33% of the total in the spent fuel⁽¹⁾, and about 113 curies of volatile solids or solid fission products (cesium compounds). This amount of volatile solids represents all of that fraction of the cesium that had migrated to the pin void spaces during reactor operation and that could conceivably be released. According to the AEC Staff, experimental data show it is unlikely that more than 1% of the total cesium in all of the fuel pins will migrate to the void space during reactor operation, and of this amount, less than 1% would be released under conditions postulated to occur in a severe transportation accident. Consequently, in the present study, the 113 curies represents all of the cesium that might be released, or about 0.01% of the total cesium in all of the fuel pins. Furthermore, it was assumed that the cesium was released as fine particles of the oxide Cs_2O at the time the pins burst and the fission gases are released.

Table i

Summary of Results: Events and Times Following a Hypothetical
Accident Involving the IF-300 Spent Fuel Shipping Cask^(a)

Event	Breach Flow Area 0.025 in ²		Breach Flow Area 0.25 in ²	
	Breach Up	Breach Down	Breach Up	Breach Down
Cask Emptied of Primary Coolant	4 Hrs 37 Min	1 Hr 56 Min	1 Hr 8 Min	16 Min
First Pins Burst (c)(d)	6 Hrs 37 Min	3 Hrs 56 Min	4 Hrs 8 Min	4 Hrs 16 Min
Last Pins Burst (c)(d)	11 Hrs 37 Min	10 Hrs 56 Min	12 Hrs 8 Min	13 Hrs 16 Min

- (a) Two different cooling times were used for the spent fuel carried in the IF-300. To be conservative with respect to the radioactivity of the fission product inventory, a cooling time of 90 days was used. The decay heat generation used was for fuel that had cooled 120 days.
- (b) Except for a small amount of residual vapor.
- (c) Fission product release times are the same as the pin burst times.
- (d) A 10-hour creep-rupture strength vs. temperature relationship was used for the Zircaloy-4 pin clads⁽⁷⁾ (see Section 3.2.1 in the Appendix). This is only temporary until the model can be modified to calculate cladding failure based on a time-temperature dependent creep-rupture technique.⁽²³⁾

Table ii

Summary of Results: Events and Times Following a Hypothetical
Accident Involving the AMCO Spent Fuel Shipping Cask^(a)

Event	Breach Flow Area 0.025 in ²		Breach Flow Area 0.25 in ²	
	Breach Up	Breach Down	Breach Up	Breach Down
Cask Emptied of Primarily Coolant ^(b)	20 Days	7.0 Hours	20 Days	43 Min
First Pins Burst ^{(c)(d)}	(e)	(e)	(e)	(e)

- (a) Two different cooling times were used for the spent fuel carried in the AMCO cask. The heat source at steady-state conditions and during coolant loss was the decay heat from fuel that had cooled 100 days. For the analyses of conditions following loss of the coolant, a decay heat was used corresponding to fuel that had cooled 120 days. The radioactivity of the fission product inventory was based on a cooling time of 120 days.
- (b) Except for a small amount of residual vapor.
- (c) Fission product release times are the same as the pin burst times.
- (d) A 100-hour creep-rupture strength vs. temperature relationship was used for the Type 316 stainless steel pin clads⁽²¹⁾ (see Section 3.2.1 in the Appendix). This is only temporary until the model can be modified to calculate cladding failure based on a time-temperature dependent creep-rupture technique.⁽²⁰⁾
- (e) None of the pins were calculated to burst, at least not up to 52 hours after the coolant was lost. At this time, temperatures in the cask appear to be approaching a new steady-state distribution.

In all the cases evaluated, the fuel temperature does not reach the vaporization temperature of the cesium (1238°F) until about 15 hours after the last of the pins burst, or about 23 to 28 hours following loss of the coolant. It should be pointed out that this release of 113 curies of cesium is to the cask containment only. The amount that might be lost through the breach has not been established but is expected to be small.

A model was developed to simulate the behavior of the aerosol formed by the fission gases and solids released from the pins. This model simulates coagulation, settling and plateout of particles in five size groups. A system of equations was developed to define the rate of flow of aerosol from the cask, but these equations were developed too late to include a leakage term in the present model. The results of the simulations show that, for all the cases evaluated, about 53% of the cesium (about 60 curies) remains suspended in the cask containment 24 hours after loss of coolant or about 9 to 13 hours after the last of the pins burst. This represents a so-called "persistent tail" composed of the smallest particle sizes considered. The pressure in the cask after the coolant is lost is near atmospheric. As the pins burst and the fission products are released and heated, this pressure will increase. This will force some of the aerosol through the damaged relief valve. The amount of cesium lost from the cask in this manner will be determined when the leakage term is included in the aerosol model.

Simulation of the behavior of the AMCO cask following loss of its primary coolant gave results indicating that the fuel in this cask might not release any of its fission products, at least not by 52 hours after the coolant is lost. At this time, the temperatures in the cask appear to be approaching a new steady-state distribution. The temperature of the hottest fuel pins is about 1397°F, but the corresponding pressure in the pins is 500 psia, compared to a pressure of about 990 psia required to burst the pin clads.

The total amount of fission gases that are free or present in the fuel pin voids and available for release is about 1537 curies, or about 56% of the total in the spent fuel. The total amount of cesium that could be released is assumed to be about 657 curies, or 0.01% of the total in the cask's load of spent fuel.

A common way to present complex interacting parts of a system's behavior is in a fault tree-type event network. Such a network was constructed for both the IF-300 and AMCO casks, based on events and their times of occurrence obtained from the cask simulations.

INTRODUCTION

This report describes the development and use of simulation models of typical LWR and LMFBFR spent fuel shipping casks to determine the quantity of fission products that might be released from these casks following a hypothetical accident and fire. It was assumed that these casks were damaged in the accident and were subsequently immersed in a petroleum fire with an effective temperature of 1475°F. The casks modeled were the General Electric IF-300, designed for the shipment of spent LWR fuel,⁽¹⁾ and a cask designed by the Aerojet Manufacturing Company (AMCO) for the shipment of spent LMFBFR fuel.⁽²⁾

A set of five simulation models has been developed for each of these casks. These models simulate cask behavior during normal operating conditions, and during conditions following an accident and fire. The sets of models include:

1. A model simulating the steady-state thermal behavior of a cask prior to an accident.
2. A model that determines the transient thermodynamic behavior of a cask and the gradual loss of primary coolant following impact and opening of a breach in the cask containment. This model applies to the case where the cask comes to rest with the breach down.
3. A model simulating the transient thermodynamic behavior of a cask and gradual loss of primary coolant following impact and opening of a breach in the cask containment. This model applies to the case where the cask comes to rest with the breach up.
4. A model simulating the transient thermal behavior of a cask following the eventual loss of primary coolant.
5. A model simulating the transient behavior of volatile solids or solid fission products (cesium compounds) that may be released to the cask containment as an aerosol at the time the fuel pins burst and the fission gases are released.

Of these models, the second, third and fifth were developed for programming on the MIMIC simulation code.⁽³⁾ The first and fourth models were programmed on the TAP simulation code,⁽⁴⁾ a network analyzer. For the IF-300, portions of the second and third models are represented by a chart devised by Moody⁽⁹⁾ relating the maximum steam and water flow rates to the local stagnation properties in a pressurized vessel. For the AMCO cask, the second model is an energy balance relating the potential energy of the coolant column to the mass velocity of the coolant flowing from the breach and the time required to empty the cask. A detailed discussion of the development of these models is presented as an Appendix to this report. Results obtained using these simulation models are presented and discussed in the next section.

In addition to these models, equations were developed to define the rate of flow of fission gases and volatile solids or solid fission products from a cask. These equations are presented in the Appendix, in the sections describing the fourth and fifth models (Sections 3.5 and 4.1.5, respectively).

The models described above have been used to estimate the amount of radioactive fission products that might be released from a shipping cask following an extremely severe hypothetical accident. These calculated estimates are presented along with some other results of the simulations that include temperatures in the casks; the rate of primary coolant loss, the internal pressures in the fuel pins, etc.

If a probability could be assigned to the sequence of events that might eventually lead to the loss of primary coolant from a cask, it would be extremely low. It has been established that the probability of a rail accident is about 10^{-8} per vehicle mile.⁽³²⁾ Further, the probability of a breach of the primary containment is very small because Nuclear Regulatory Commission (NRC) standards require that all licensed casks withstand severe drop and puncture conditions.⁽⁵⁾ Combining these low probabilities results in an even lower probability that the cask containment would ever be breached.

The General Electric Company made a study of a hypothetical accident as part of the design and safety analysis of its IF-300 Spent Fuel Shipping Cask.⁽¹⁾ For this analysis, General Electric assumed that the water in the neutron shield was lost at the time of the accident, and that the primary coolant in the cask cavity was then gradually lost through a series of relief valve blowdowns as the temperatures in the cavity increased. This analysis, in which the pressure relief valve was assumed to be functioning properly, demonstrated that the radioactivity of the coolant released was within the limits specified in Section 71.36(a)(2) of the Code of Federal Regulations (10CFR71).⁽⁵⁾

Analytical tools to predict cask behavior under simulated accident conditions should assist in the design of casks to withstand severe accidents. The development of the cask simulation models and the construction of an event diagram (Figure 26) displaying alternate paths leading to fission product release should be of value to cask designers.

The simulation of cask behavior helps to assure cask integrity and, consequently, the protection of the surroundings under accident conditions. Certain events may occur in a spent fuel shipping cask, following an accident and fire, that might lead to the release of fission products. If these events can be identified in advance through simulation, and steps taken to delay or prevent their occurrence, the safety and integrity of the cask design will be significantly increased.

The simulation models developed provide the means for answering two very important questions that should be asked when planning remedial procedures to be implemented in the event of an accident involving a spent fuel shipping cask. These questions are:

1. How much time would be available to evacuate personnel from the area after the accident if the same damage and arbitrarily selected breach-causing mechanism used in the simulation were assumed for the actual accident?

2. How much time would be available for putting corrective measures into effect before radioactivity is released or before radiation shielding is reduced?

The results of this study provide some answers to these questions (see Results of the Simulations, parts B and C, in the next section, and the section on Conclusions and Recommendations).

RESULTS AND DISCUSSION

Cask Descriptions and Data

The LWR spent fuel shipping cask analyzed is the General Electric IF-300 design presented in General Electric drawing 159C5238 in Reference 1. Figures 1 and 2 are copies of portions of this drawing. Detailed data on this cask are presented in Table 1.

The IF-300 carries seven PWR fuel assemblies. These assemblies are surrounded by slotted stainless steel baskets. Several stainless steel-boron carbide rods are attached to the outer surfaces of the baskets for criticality control (see Figure 3). The seven assemblies and their baskets are contained in an inner cavity or containment vessel, which is cooled by water and surrounded by four inches of depleted uranium shielding encased in stainless steel. The outer surface of the uranium is cooled by water contained in a six-inch jacket. The type of fuel assembly that would be carried by this cask is shown in Figure 4.⁽⁸⁾ Detailed data on this fuel assembly are presented in Table 2.^(1,8)

The LMFBR spent fuel shipping cask analyzed is one designed by the Aerojet Manufacturing Company (AMCO) for FFTF and LMFBR demonstration plant use.⁽²⁾ This cask is shown in Figure 5, and detailed data are presented in Table 3.^(2,11) Although this cask has been designed for shipment of FFTF and LMFBR demonstration plant spent fuel, it will be referred to throughout this report as an LMFBR spent fuel shipping cask.

The AMCO cask of Figure 5 carries nine fuel assemblies. Each of these nine hexagonal fuel assemblies is enclosed in a steel basket with slots for coolant flow. The nine assemblies and their baskets are contained in a stainless steel canister cooled by either Dowtherm-A or sodium. Dowtherm-A was selected as the coolant for this study. The fuel assemblies are arranged in a circular pattern, bounded on the inside by an expansion chamber shell with an outer diameter of 15.5 inches, and bounded on the outside by the inner wall of the canister. The canister has a one-inch thick wall, separated from the inner wall of the containment vessel by a 0.25-inch helium filled gap. The containment vessel is surrounded by a 3.625-inch thick

CAVITY RELIEF VALVE
TARGET ROCK CORP
600# ANSI 350
PSIG SET PRES.

VIEW D-D
SHOWING UPPER CASK
VALVE BOX

VIEW C-C
SHOWING BARREL VALVE
BOX (TYP 2 PLCS)

RELIEF VALVE
MPCO# 5-1SF
(SETTING 200 PSIG)

VIEW B-B
SHOWING LOWER CASK
VALVE BOX

1 IN. SST BELLOWS
SEAL GLOBE VALVE

SECTIONAL VIEW OF CASK WITH PWR CASK HEAD

HEDL 7507-30.57

FIGURE 1. General Electric IF-300 LWR Spent Fuel Shipping Cask

HEDL 7507-30.58

FIGURE 2. General Electric IF-300 LWR Spent Fuel Shipping Cask (Page 1 of 2)

FIGURE 2. General Electric IF-300 LWR Spent Fuel Shipping Cask. (Page 2 of 2)

TABLE 1

Characteristics of Design Basis PWR 1 Fuel
and General Electric IF-300 Spent Fuel Shipping Cask

Fuel

Type	PWR
Exposure, GWd/MTU (average)	35.0
Operating Power, kW/kgU	40.0
Assembly Heat Power, W/kgU	24.03
Assemblies per Cask Load	7
Uranium, kgU/Assembly	457
Maximum Decay Heat Rate-Cask, Btu/hr	262,000 *
Number of Fuel Rods/Assembly	205

Cask

Cavity Length, ft	14.104
Cavity Diameter, ft	3.1250
Inner Shell Thickness, ft	0.0417
Shielding Thickness, ft	0.3333
Outer Shell Thickness, ft	0.1250
Cask Linear Surface Area, ft ² /ft	32.2
Cask Length, Excluding Fins, ft	15.844
Cask Cavity Water, lb	4800
Shielding Water, lb	4540
Cavity Relief Pressure, psig	350
Exterior Containing Relief Pressure, psig	200

Cooling System

Cooling Medium	Forced Air
Number of Full-Length Cooling Nozzles	4
Cooling Air Arrival Velocity, fps	47.0
System Classification	Open
Surface Film Coefficient, Btu/hr-ft ² -°F	7.0
Minimum Air Flow, cfm	10,000

* This value was used in this study and by GE⁽¹⁾ to be conservative. It is 25% higher than the heat rate sanctioned by the Nuclear Regulatory Commission.

1. OUTER LINER
2. SHIELD
3. INNER LINER
4. WATER
5. CHANNEL
6. B₄C POISON RODS
7. FUEL BUNDLE (PWR)

NOTE: 14 GAGE SHEET = 0.0747 INCH THICK

HEDL 7507-30.18

FIGURE 3. Arrangement of PWR Spent Fuel Assemblies in the IF-300

HEDL 7507-30.3

FIGURE 4. LWR Fuel Assembly

TABLE 2

Characteristics of Design Basis PWR 1 Fuel
(Compiled from data obtained from References 1 and 8)

Fuel Pin

Fuel Pellet Diameter, in	~0.420
Fuel Pellet length, in	0.6
Fuel Pellet Density, gm/cm ³	10.19-10.3
Cladding Thickness, in	0.020
Cladding Outside Diameter, in	0.460
Active Fuel Length, in	144.
Length of Gas Plenum, in	~ 4.0
Fuel Material	Sintered UO ₂
Cladding Material	Zircaloy-4

Fuel Assembly

Fuel Pin Array	15 x 15
Pins per Assembly	205
Fuel Pin Pitch, in	0.582
Overall Dimensions, in (Slotted envelope)	8.75 x 8.75
Weight of Uranium per Assembly, Kg	457.
Assembly Cooling Time, days	120
Assembly Heat Generation, Watts/KgU	24.03

HEDL 7507-30.59

FIGURE 5. AMCO LMFBR Spent Fuel Shipping Cask (Reference 2) (Page 1 of 3)

FIGURE 5. AMCO LMFBR Spent Fuel Shipping Cask (Page 2 of 3)

HEDL 7507-30.61

FIGURE 5. AMCO LMFBR Spent Fuel Shipping Cask (Page 3 of 3)

TABLE 3

Descriptive Data on the AMCO LMFBR Spent Fuel Shipping Cask
(References 2 and 11)

Typical Fuel Properties - FFTF Fuel

Elements per cask	9
Mass of fuel, kg (U + Pu)	280
Burnup, MWD/MT*	
Peak	80,000
Operating	75,000
Average	50,000
Specific Power, MW/MT	159.1
Decay Time, days	100
Radioactivity, megacuries	-
Thermal power, Kw	19.8

Cask

Cavity diameter	32.25
Cavity length, ft	14
Inner shell thickness, in	1
Gamma shell thickness, in	3.625 U
Outer shell thickness, in	6.0 Steel
Neutron shield thickness, in	4
Outer liner thickness, in	~ 0.25
Fin height, in	8
Overall diameter, in	78.5
Overall length, ft	18.67
Internal coolant	Dowtherm-A
Shield Coolant	water

* MT = Metric Ton

uranium shield which, in turn, is surrounded by a 6-inch thick steel shell. The outer surface of the steel shell is cooled by water contained in a four-inch jacket partitioned by circumferential cooling fins extending through the jacket and protruding eight inches beyond the outer diameter of the jacket. The fuel assembly carried by this cask is shown in Figure 6, and detailed data are presented in Table 4.

A simplified model of the IF-300 is shown in Figures 1-1, 1-3, 3-1, 3-2, 3-19 and 3-20 in the Appendix. The primary difference between this model and the actual cask is the representation of the fuel, cans and baskets as circular regions rather than the array of square fuel assemblies. A collection of fuel pins have a "lumped" characteristic. It was necessary to devise a method of "distributing" the "lumped" fuel to give homogeneous regions that could then be relumped to fit the nodal representation of a simulation network. The techniques for doing this are discussed in detail in the Appendix.

A simplified model of the AMCO cask is shown as a simulation network or electrical analog in Figures 1-2 and 3-21 in the Appendix. This model represents one-ninth of the cask cross-section, a pie-shaped slice containing one fuel assembly. As in the case of the LWR fuel assembly, the collection of LMFBR fuel pins in an assembly were distributed to give a homogeneous region and then relumped to fit the nodal representation of the simulation network.

These simplified models of the casks were used to simulate the steady-state conditions in the casks before the accident, and the thermal behavior of the casks following an accident, fire, and eventual loss of the primary coolant. Other models of the casks, even simpler and less detailed than those listed above, were used to simulate the thermal behavior of the casks during the fire following the accident, with gradual loss of primary coolant through a breach in the cask containment. These cask models are shown in Figures 2-4 and 2-7 in the Appendix.

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FIGURE 6. FFTF Driver Fuel Assembly

TABLE 4

Data for FFTF Reactor Core

FFTF Driver Fuel Pin, Cold

Fuel pellet diameter, in	0.196
Fuel pellet length, in	0.25
Fuel pellet density, gms/cm ³	10.
Cladding thickness, in	0.015
Cladding outside diameter, in	0.23
Active fuel length, in	36.
Length of gas plenum, in	42.
Fuel material	PuO ₂ -UO ₂
Cladding material	SS-316
Number of fuel pins	16,492

FFTF Fuel Assembly

Number of fuel assemblies	76
Fuel pin array	Hexagonal-6 rows
Pins per assembly	217
Fuel pin pitch, in	0.286
Overall dimensions, in	4.7 across flats
Weight of PUO ₂ -UO ₂ per fuel assembly, lbs	88.6
Fuel channel material	SS-316
Wire wrap-wire diameter, in	0.056

Fission Product Release Mechanisms

Several fission product release mechanisms have been postulated or identified, and some have been evaluated. The bulk of the fission products released are fission gases and volatile solids or solid fission products (cesium compounds). Before discussing release mechanisms it is necessary to define what is meant by "free" gases and "bound up" gases. Fission gases and volatile solids generated during reactor operation either migrate to the fuel pin voids (the spaces between the clad and the fuel, the spaces between the fuel pellets, and the plenum space or expansion chamber at the end of the fuel pin), or remain inside the fuel material. Those fission gases and vapors migrating to the pin voids are "free". The remaining fission gases and vapors produced are bound up in the interstices of the fuel material, hence the term "bound up".

Some possible mechanisms for fission product release from the fuel to the cask containment are:

1. Clad rupture that releases the free fission gases and solid fission products from the fuel pin voids and exposes the fuel to the environment in the containment vessel.
2. Diffusion of bound up fission gases and volatile solids from the fuel, if the temperature is high enough. This is negligible for the times and temperatures encountered in the accident analysis.
3. Disintegration of the fuel upon oxidation that releases bound up fission gases and volatile solids. The exposed fuel oxidizes during the same time it is capable of losing bound up fission gases by diffusion. When oxidation progresses to the point where the fuel undergoes a phase change upon conversion to U_3O_8 , a loose granular material, the bound up fission products are assumed to be released. Results obtained using the simulation models indicate that the cask interior is always at a higher pressure than the surroundings;

therefore the chances of air entering the containment vessel are considered to be very low. The only time oxidation would be an important release mechanism would be in the unlikely event that massive damage would be suffered by the casks and the fuel would become directly exposed to the environment. Oxidation of the fuel by the water vapor remaining in the IF-300 after loss of coolant, to the extent required to release substantial amounts of fission products, is considered to be unlikely.

4. The radioactive crud entrained in the primary coolant will be lost from the cask in the event of coolant loss. When the fuel assemblies are placed in the shipping cask, there will be a certain amount of radioactive residue or "crud" adhering to the surfaces of the assemblies.

Fission products may be released from the cask containment by leakage from some breach in the cask containment. As stated earlier, the breach in the cask containment was arbitrarily assumed to be due to a damaged pressure relief valve. This was an arbitrary assumption for the purpose of this study and must not be interpreted as an implication that the pressure relief valve is vulnerable to damage or malfunction. On the contrary, the relief valve is not only a well designed and proven component, but is also extremely well protected in the IF-300 design (see Figures 1 and 2). The escape of nonvolatile fission products or of transuranium isotopes would require the assumption of extremely severe conditions, including extensive mechanical damage to the fuel.

Results of the Simulations

Some radioactivity in the form of crud, fuel particles, and some free fission gases from damaged fuel pins could be released immediately after impact as the primary coolant is lost. It was estimated that about 1.6 curies could be released as crud. The amount of radioactivity released at impact as fuel particles and free fission gases requires some knowledge

of the extent of damage to the fuel pins, and of the mechanism of escape of the fuel particles from the damaged pins and their subsequent dispersion in the coolant. A reasonable estimate of the number of pins breached at impact may be obtained from a mathematical model simulating the mechanical response of the fuel assemblies to the impact force, or from an equivalent experimental program. A model simulating this event in the accident sequence has not yet been developed for this study; however, similar studies in the past have led to the development of some preliminary models that simulate the elastic-plastic response of structures to an impulse such as that which might be experienced by the fuel assemblies at impact.⁽³⁴⁾ Experience gained from this earlier work is directly applicable to the development of a mechanical response model for the fuel assemblies. The release of fuel particles and free fission gases will be delayed if the fuel pin clads do not fail at impact.

Although the extent of damage to the fuel pins at impact has not yet been determined, and the exact amount of fission products released cannot be reliably estimated, some indication of how these events may be factored into the present analysis is offered through the following scenario. If all or a fraction of the pins are ruptured at impact, fission products will be released. Fission gases would probably be released through any breach in the cladding, but particulate matter would only be released through those openings large enough to accommodate at least the smallest particles formed. Upon release, the fission gases would rise through the primary coolant to the top of the cask cavity, while the fine particles of solid material would be suspended and dispersed in the coolant and the larger particles would settle to the bottom of the cavity. If the cask is in a breach up position after impact, the fission gases will escape through the breach. Also, some fine solid particles may be entrained in the coolant vapor flowing through the breach. However, the larger particles, which have settled to the bottom of the cavity, would remain in the cask even after the cask has lost all coolant. If the cask is in a breach down position after impact, the fission gases will not be released until after the cask has been emptied of its liquid primary coolant. The fission gases will mix with the vapor phase primary

coolant above the liquid. The fine solid particles suspended and dispersed in the liquid coolant would flow from the breach along with the coolant. The larger solid particles at the bottom of the cavity may be swept into the breach along with the coolant. If the breach is small enough, and the particles large enough, the particles may clog the breach and prevent further loss of coolant and fission products (especially if the cask is designed with an in-line filter). If the particles cannot completely clog the breach, the cask will eventually lose all its liquid coolant, and the vapor-fission gas mixture will flow through the breach. Some fission gases will remain in the cask, along with residual vapor, when the pressure inside the cask decreases to atmospheric pressure. Some elements of the analytical approaches presented in Sections 2, 3.5 and 4 in the Appendix may be used to help in any simulation of the events described in the above scenario. If it can be established that some fraction of the pins have been ruptured at impact, the behavior of the remaining undamaged pins would be simulated using the models developed for the study of this report.

A list of simulation models developed for this study has been presented and briefly discussed in the Introduction. This list includes a set of five simulation models for the IF-300 and a similar set of models for the AMCO cask. These models simulate cask behavior during normal operating conditions, and during conditions following an accident and fire. The development of each of these models is discussed in detail in the Appendix. Results obtained using these models will now be presented and discussed.

A. Steady-State Temperatures in the Casks Before the Accident

The steady-state temperatures in the casks before the accident were determined to establish initial conditions for the post-accident transient analyses to be discussed later. Details of the steady-state simulation models of the casks are discussed in Section 1 of the Appendix. These models simulate conditions in the casks while in transit, during an uneventful, normal trip.

In both casks, decay heat generated by the spent fuel is transferred by natural convection to the primary coolant inside the fuel assembly cans, which in turn transfers the heat to the inner wall of the cans. The heat is then conducted through the can walls to the outer surface, where it is then transferred by natural convection to the primary coolant outside the fuel assemblies. The primary coolant outside the fuel assemblies then transfers the heat to the inner wall of the containment vessel, also by natural convection. The heat is then transferred by conduction through the steel liners and shielding of the cask wall, and by radiation and conduction across any small gaps. At the outer liner, some of this heat is transferred to the water in the outer jacket by natural convection. The AMCO cask design includes circumferential fins, which are attached to the outer liner and extend through the jacket to protrude eight inches beyond the outer shell of the jacket. These fins pick up some of the heat transferred to the water in the outer jacket, along with heat conducted through the fins from the outer liner. Heat is transferred from the fins and from the outer shell of the water jacket to the surroundings by natural convection and radiation. The IF-300 design does not have fins attached to the outer liner, which extend into and through the water jacket. Instead, the outer surface of the water jacket is corrugated, and air is forced over the outside of the corrugated surface to dissipate the heat transferred into the water jacket. Both casks are covered by a solar shield while in transit.

The coolant circulation patterns and heat transfer paths in the cavities in the casks, which contain the spent fuel, are discussed in Section 1.1 of the Appendix.

A collection of fuel pins, such as those in the fuel assemblies, have a "lumped" characteristic. A method was devised to "distribute" the "lumped" fuel to give homogeneous regions that could then be "re-lumped" to fit the nodal representation of the models. This was done by using the concepts of volumetric heat dissipation and an apparent thermal conductivity for materials with voids to represent the heat transfer in the fuel regions. The equations defining these concepts are presented in Sections 1.2 and 1.3, respectively, in the Appendix.

The steady-state temperatures in the IF-300, obtained for the conditions specified in Tables 1 and 2, are shown in Figure 7. The maximum fuel temperature is 361°F, the water in the cask cavity is about 333°F, and the water inside the fuel cans is at about 360°F. The calculated fuel temperature is about 44°F higher than that reported in Reference 1, and the temperature of the water in the cask cavity is about 30°F higher. Temperatures obtained from Reference 1 are also shown in Figure 7. The General Electric study of Reference 1 was based on a two-dimensional model that considered heat flow from the ends of the cask, as well as that which flows radially from the cask. The present study was based on a one-dimensional model where only heat flow from the cask in the radial direction was considered. This might account for the differences in the results.

Steady-state temperatures in the AMCO cask, obtained for the conditions specified in Tables 3 and 4, are shown in Figure 8. The maximum fuel temperature is 383°F, and the Dowtherm-A in the cask cavity is at a temperature of about 343°F. The fuel temperature is about 20°F higher, and the temperature of the coolant in the cask is only 2°F lower than the corresponding temperatures reported in Reference 2. The temperature of the coolant inside the fuel assembly cans was not reported in Reference 2. Temperatures obtained from Reference 2 are also shown in Figure 8.

B. Analyses of Rate of Coolant Loss from the Casks

Analyses were made for both the IF-300 and the AMCO casks in an effort to estimate realistic coolant loss rates. This was an important phase of the study because if it could be shown that the rate of coolant loss was low enough and the cask could be approached after the fire ends, before a substantial amount of coolant was lost, then steps could be taken to restore the cask to near pre-accident conditions. Results of these analyses show that, although the loss of the coolant is not instantaneous, the time required to empty the IF-300 is small enough, in all of the cases considered, to rule out any thought of restoring this cask to near pre-accident condi-

FIGURE 7. Steady-State Temperatures in the IF-300 Before the Accident

FIGURE 8. Steady-State Temperatures in the AMCO Cask Before the Accident

tions. However, results show that there is ample time to restore the AMCO cask to near pre-accident conditions in two of the four cases considered.

It was assumed that the primary coolant would be lost from the casks through a damaged or malfunctioning pressure relief valve. There are two possible ways in which the primary coolant may be lost from a breached cask. These depend upon the final orientation of the cask after the accident. At impact, if the tiedowns fail, the cask may become separated from the rail car and come to rest in one of four positions:

1. On end with the breach (damaged relief valve) up,
2. On end with the breach down,
3. On its side with the breach up, and
4. On its side with the breach down.

If the tiedowns do not fail at impact, the cask will remain in its original orientation on the rail car, i.e., on its side as in positions 3 and 4 above. The first mechanism for coolant loss depends on the cask being oriented in positions 2 and 4. In these positions, the coolant may leak out under the driving force of its own liquid head and the static pressure in the cask. The second mechanism for coolant loss depends on the cask being oriented in positions 1 and 3. In these positions, the coolant would not leak out, but would escape from the cask by vaporization as it absorbs the decay heat from the fuel.

A model was developed to simulate the transient thermodynamic behavior of the IF-300 and to determine the time required for it to lose its primary coolant. This model is based on energy and mass balances on the cask, and on an energy balance on the coolant flowing through the breach. The main driving force that causes the coolant to flow from the cask through the breach is the buildup of static pressure in the cask cavity. This pressure buildup is partly due to that portion of the decay heat from the fuel stored in the liquid and vapor phases of the coolant during the transient, and partly due to the choked flow in the breach. A detailed discussion of the development of a breach down version of this model is presented

in Section 2.1.1 in the Appendix, and the breach up version of the model is discussed in Section 2.1.2.

Two breach sizes or flow areas were assumed. The smallest flow area assumed was 0.025 in^2 , a reasonable area for a relief valve that is not fully reseated. The largest flow area assumed was 0.25 in^2 , a reasonable area if the relief valve is sheared off. Additional damage assumed to be suffered by the cask in the accident included loss of the solar shield, and rupture of the outer water jacket with immediate loss of the water. It was also assumed that the cask was immersed in a fire at a temperature of 1475°F for 0.5 hour, as specified in the Code of Federal Regulations.⁽⁵⁾

If the IF-300 comes to rest with the breach up, only vapor will escape through the gap. If the cask comes to rest with the breach down, only liquid will escape from the gap. The initial temperatures of the fuel, fuel cans, coolant and baskets in the IF-300 at the time of the accident were determined using the steady-state pre-accident model, as were the temperatures of the cask wall and surface. This steady-state model is similar to the loss-of-coolant model to be discussed later, except that the primary coolant is not lost, the solar shield remains intact, and no water is lost from the neutron shield (outer water jacket). The initial temperatures of the fuel, coolant inside the fuel cans, fuel cans and coolant outside the fuel cans at impact were 361°F , 360°F , 350°F and 333°F , respectively. An average of the coolant temperatures, 347°F , was used as the initial coolant temperature in the simulation model that determines the rate of coolant loss. The water coolant is a saturated liquid at this temperature, with a corresponding saturation pressure of 130 psia. Since this saturation pressure is about 9 times atmospheric pressure, the cask was treated as a pressure vessel. The heat source in the cask in the steady-state analysis, and in subsequent transient analyses, was the decay heat from fuel that had cooled 120 days prior to shipment.

A set of charts has been developed by Moody⁽⁹⁾ to provide a convenient method for evaluating the maximum rate of loss of steam or water from a pressurized vessel that suffers a sudden break in its containment. The maximum rate of loss of either the vapor or the liquid from the breach

is governed by a thermodynamically defined critical or maximum mass flow rate based on isentropic flow of the fluid from the breach. A chart from Reference 9, presented as Figure 2-1 in the Appendix, relates the critical or maximum mass flow rate of steam and water to the stagnation enthalpy and pressure. This chart will be referred to as the "Moody chart" throughout this report. When the mass velocity is multiplied by the area of the breach produced at impact, the rate of coolant loss is obtained.

Results show that if the IF-300 comes to rest with the breach up, it would take about 68 minutes to empty the cask of its coolant if the breach flow area is 0.25 in^2 , and about 4.62 hours if the flow area is 0.025 in^2 . In the breach-up position, only the vapor produced by boiling of the coolant can escape. At the largest flow area, the pressure in the cask builds up to a maximum of 732 psia and then decreases to atmospheric pressure. The maximum mass velocity in the breach at the peak pressure (as obtained from the Moody chart) is $1471 \text{ lb}_m/\text{sec-ft}^2$. At atmospheric pressure, 2.2 pounds of vapor remain in the cask. At the smallest flow area, the pressure in the cask reaches a maximum of about 1823 psia and then decreases to atmospheric pressure. The maximum mass velocity in the breach at this peak pressure is about $4468 \text{ lb}_m/\text{sec-ft}^2$. For this case, at atmospheric pressure, 2.0 pounds of vapor are left in the cask. In both cases, the peak pressure occurs at the instant just before all of the liquid coolant disappears, leaving only the vapor phase. Pressures in the IF-300 as functions of time, for the breach up cases, are presented in Figure 9. The corresponding temperatures in the cask are presented in Figures 10 and 11, and the masses of liquid coolant in Figure 12.

If the cask comes to rest in a breach down position, only saturated liquid would escape from the breach. Under these conditions, results indicate it would take about 16 minutes to empty the cask if the breach flow area is 0.25 in^2 and about 1.94 hours if the flow area is 0.025 in^2 . At the largest flow area, the pressure reaches a maximum of about 177 psia before decreasing to atmospheric pressure. The mass velocity in the breach at the peak pressure is greater than $3412 \text{ lb}_m/\text{sec-ft}^2$, the maximum obtained from the Moody chart for the saturated liquid, so the flow of the two-phase fluid

FIGURE 9. Cavity Pressure in the IF-300 as a Function of Time After the Accident

FIGURE 10. Temperatures in the IF-300 During Loss of Coolant (Breach Up Position, Breach Area=0.25 Sq. Inches)

FIGURE 11. Temperatures in the IF-300 During Loss of Coolant (Breach Area=0.025 Sq. Inches, Breach Up Position)

FIGURE 12. Mass of Liquid Coolant Remaining in the IF-300 As a Function of Time After the Accident

from the breach is choked. At atmospheric pressure, 2.6 pounds of vapor remain in the cask. At the smallest flow area, the pressure peaks at about 1080 psia and then decreases to atmospheric. The maximum mass velocity at this peak pressure is greater than $7470 \text{ lb}_m/\text{sec-ft}^2$, the maximum obtained from the Moody chart. In this case, 2.1 pounds of vapor are left in the cask. As before, the peak pressure occurs just before all of the liquid coolant disappears, leaving only the vapor phase. Pressures as functions of time, for the breach down cases, are presented in Figure 9. The corresponding temperatures in the cask are presented in Figures 13 and 14, and the masses of liquid coolant in Figure 12.

Initial temperatures in the AMCO cask were determined in the same manner as those for the IF-300. A steady-state pre-accident analysis indicated that the fuel, the coolant inside the fuel cans, fuel cans, and coolant outside the fuel cans were at temperatures of 383°F, 380°F, 364°F and 343°F, respectively, at the time of impact. An average coolant temperature of 360°F was used as the initial coolant temperature in the model that determines the rate of coolant loss. The model used to determine the steady-state temperatures in the cask is similar to the loss-of-coolant model to be discussed later, except that the primary coolant is not lost, the solar shield remains intact, and no water is lost from the neutron shield (outer water jacket).

The heat source in the AMCO cask was the decay heat from fuel which had cooled 100 days prior to shipment. For the analysis of conditions in the cask after it had been emptied of its coolant, a decay heat corresponding to fuel that had cooled 120 days was used. The same damage was assumed for the AMCO cask as was assumed for the IF-300, i.e., the solar shield was lost, the outer water jacket was ruptured, and a breach was opened in the cask containment. In addition, a 0.5-hour fire at 1475°F, as specified in the Code of Federal Regulations,⁽⁵⁾ was assumed.

The primary coolant in the AMCO cask is Dowtherm-A, which is a low vapor pressure coolant. Its saturation temperature at atmospheric pressure is 494.8°F.⁽⁹⁾ The average initial temperature of the Dowtherm-A coolant at the time of the accident is about 360°F, as calculated using the steady-

FIGURE 13. Temperatures in the IF-300 During Loss of Coolant (Breach Area=0.25 Sq. Inches, Breach Down Position)

FIGURE 14. Temperatures in the IF-300 During Loss of Coolant (Breach Area=0.025 Sq. Inches, Breach Down Position)

state pre-accident model. This means that the coolant is subcooled and not at saturation conditions as is the water in the IF-300. Since the pressure in the AMCO cask is about the same as atmospheric pressure at the time of impact, the rate of loss of the coolant from the breach was determined by methods different than those used for the IF-300.

A model was developed to simulate the transient thermal behavior of the AMCO cask and to determine the time required for it to lose its primary coolant, if it becomes separated from the rail car and comes to rest in a breach up position. This model is primarily a heat transfer model that simulates the thermal behavior of the cask after it has lost its solar shield and the water in its outer jacket or neutron shield. This model also applies to the case where no breach is opened in the cask containment at impact. A detailed discussion of the development of this model is presented in Section 2.2.2 in the Appendix. Results obtained from this model show that, for both the breach sizes considered, it would take about 20 days to empty the cask of its coolant if the cask breaks loose from the rail car and lands in the breach up position. This time is extrapolated from the results presented in Figure 15, since the actual computations were only carried out to about 13 days. It takes about 5.4 days for the Dowtherm-A to absorb the heat required to reach its saturation temperature of 494.8°F. At this point, the coolant boils and leaves the cask as vapor. By 12.8 days, 1616 pounds or 42.6% of the total 3790 pounds of coolant has boiled away (see Figure 15). A straight line extrapolation of the curve of coolant mass remaining would give a conservative estimate of about 20 days for the cask to empty completely. The coolant leaves the cask as vapor with a maximum mass velocity of about $130 \text{ lb}_m/\text{sec-ft}^2$ at a breach area of 0.025 in^2 , the smallest breach size considered.

A different model was developed to estimate the rate of coolant loss from the AMCO cask and the time required to lose all of its primary coolant if it comes to rest in a breach down position. This model was based on an energy balance relating the isentropic flow of Dowtherm-A through the breach to the potential energy of the coolant column. The development of this model is discussed in detail in Section 2.2.1 in the Appendix.

FIGURE 15. Behavior of the AMCO Spent Fuel Shipping Cask Following an Accident and 0.5 Hour Fire (Gradual Loss of Primary Coolant)

Results from this model show that at impact, when the Dowtherm-A is at an average temperature of 360°F, it would take about 43 minutes to empty the cask if the breach area were 0.25 in² and about 7.0 hours if the breach area were 0.025 in².

The results from these models indicate that there may be ample time to restore the AMCO cask to near pre-accident conditions if the cask comes to rest in the breach up position after the accident, regardless of the breach sizes considered. However, the results also show that, if the cask comes to rest in the breach down position and if the breach flow area is 0.25 in², there would not be enough time available to restore the cask to near pre-accident conditions before the bulk of the coolant is lost. If the breach flow area is 0.025 in², enough time might be available to take some remedial action.

The model of the AMCO cask used to determine the rate of loss of coolant from the cask when it comes to rest in a breach up position was also used to simulate the transient behavior of the cask for various other post-accident cases. These post-accident cases were based on the common assumption that no breach was opened at impact. In one such case investigated, it was assumed that the only damage to the cask at impact was the loss of the solar shield and the loss of the water in the outer jacket. For these conditions, the cask reached a new steady-state condition in about 6.5 days (see Figure 16). The coolant temperature at this new steady-state condition oscillates between 501°F and 499°F due to the diurnal variation of solar heating. The saturation pressure at 500°F is 15.7 psia, 1.0 psia above atmospheric. The Dowtherm-A volume expands about 9.5% in going from an initial temperature of 343°F to the final temperature of about 500°F; however, it was estimated that the cask could withstand a 16% coolant volume expansion.

Another case was studied in which it was assumed that the water in the outer jacket was lost, but that either the solar shield remained intact, or a solar shield was jury-rigged as soon as the fire died and the cask could be approached. Results for this case indicated that the cask approached a new steady-state condition in about 8 days when it began leveling off at a coolant temperature of 481°F. In the next 4.5 days (for a total of

FIGURE 16. Behavior of the AMCO Spent Fuel Shipping Cask Following an Accident and 0.5 Hour Fire (No Loss of Coolant)

12.5 days) the coolant temperature only rose another 0.6°F (see Figure 17). This temperature is well below the saturation temperature. For this case, the coolant volume expands by about 8.4%. The length of the fire at the time of the accident does not appear to have a significant effect on the thermal behavior of the cask, at least for fires up to 2.0 hours duration. Calculations were made for no fire, a 0.5-hour fire, and a 2-hour fire, with no visible difference in the results.

The oscillatory nature of the coolant mass curve in Figure 15 (and the temperature curves in Figures 15 and 16) is due to the diurnal variation of the solar heat input to the cask. During the 12 hours of daylight, solar heat is added at the rate of 19.5 BTU/sec, which is enough to maintain the vaporization of the Dowtherm-A once it has reached its saturation temperature. During the 12 hours of night, with no solar heat input, the rate of coolant boiloff tends to level off at a level consistent with the improved conditions for heat loss from the cask. A further indication of the sensitivity of the behavior of the AMCO cask to solar heat input is apparent by comparing the results presented in Figures 16 and 17. Figure 16 illustrates the behavior of the cask if the only damage suffered at impact was loss of the solar shield and of the water in the outer jacket, but with no loss of Dowtherm. Figure 17 reflects the behavior of the cask for the same conditions, except that the solar shield either remains intact or a substitute shield is jury-rigged as soon as the fire is out. Without a solar shield, the temperatures oscillate due to the diurnal variation of the solar heating. With the solar shield, the results do not have this oscillatory characteristic and the coolant temperature levels off at about 20 degrees less than that obtained without the solar shield, and about 13 degrees below the saturation temperature of 494.8°F at atmospheric pressure.

Solar heat input, as can be seen from these results, is an important factor. The total solar heat input during the day is 19.5 BTU/sec, as compared to a total decay heat generation in the fuel for the AMCO cask of 19.0 BTU/sec. The difference is that the solar heat is applied to the

FIGURE 17. Behavior of the AMCO Spent Fuel Shipping Cask Following an Accident and 0.5 Hour Fire

external surface of the cask where it only affects the external surface sink temperatures, while the decay heat is generated at the very heart of the cask internals and must flow to the surface. Some of this decay heat is absorbed by the internals (including the coolant) during the transient, which increases their temperatures. The question could be asked: If the solar heat input is so important and influential, why is the fire of so little consequence? The answer is that the fire, although at the high temperature of 1475°F, is of a very short duration, 0.5 to 2.0 hours, compared to the 12.0 hours at a time that the solar heat is applied. The solar heat input to the cask varies from 0 BTU/sec at night to 19.5 BTU/sec during the day.

If either the IF-300 or AMCO cask comes to rest on its side after impact, or remains in this position on the rail car, the time to lose the primary coolant would probably fall somewhere near the times estimated for the positions already evaluated, depending on the final orientation of the breach.

C. Analysis of Fission Product Release Following Loss of Coolant

Simulation of the behavior of the IF-300 following emptying or loss of its primary coolant gave results that indicate that this cask might release about 11,900 curies of fission gases, about 33% of the total fission gases in the spent fuel (see Figures 18 and 19). According to Reference 1 (Tables IX-8 and IX-9), this is the total amount of free fission gases present in the fuel pin voids and available for release. This represents about 35% of the Kr-85 and I-129, and about 3% of the Xe and I-131 in the cask's 3.2 MT of spent fuel.

While the primary coolant is being forced from the IF-300, and after the cask has lost its coolant (except for some residual steam), the fuel pin temperatures increase. Eventually, these increasing temperatures cause the pin clads to burst due to the expansion of free fission gases in the pin voids. The fission gases would then be released along with some particulate matter. At this time, until a time-temperature dependent

FIGURE 18. Total Radioactivity Released as Fission Gases from the Spent Fuel in the IF-300 (Breach Up Position, Breach Areas of 0.25 and 0.025 Sq. Inches)

FIGURE 19. Total Radioactivity Released as Fission Gases from the Spent Fuel in the IF-300 (Breach Down Position, Breach Areas of 0.25 and 0.025 Sq. Inches)

creep-rupture technique ⁽¹⁹⁾ can be adapted to the models, the strength of the clads is assumed to follow a creep rupture strength vs. temperature relationship (see Section 3.2.1 in the Appendix).

Results of this simulation show that the temperature at which the fuel pin clads burst is about 921°F, which corresponds to an internal pressure of about 1896 psia. For the breach flow area of 0.25 in², with the cask in the breach down position, the first pins burst 4.27 hours after impact (4.0 hours after loss of the primary coolant). For this case, the last of the pins burst at 13.27 hours after impact (13.0 hours after loss of coolant). For the same breach flow area, but with the cask in the breach up position, the first pins burst 4.13 hours after impact (3.0 hours following loss of coolant) and the last of the pins burst 8.0 hours later at 12.13 hours (11.0 hours after loss of coolant). At the smaller breach flow area of 0.025 in², with the cask in the breach down position, the first pins burst 3.94 hours after impact (2.0 hours after loss of coolant) and the last pins burst at 10.94 hours after impact (9.0 hours after loss of coolant). At this same flow area, but with the cask in the breach up position, the first pins burst 6.62 hours after impact (2.0 hours after loss of coolant).

Temperatures in the IF-300 following loss of primary coolant are presented in Figures 20, 21, and 22 for the case where the cask has a breach flow area of 0.25 in² and is in the breach down position. These temperatures are the only ones plotted and were chosen because, among the four cases considered, this was the only one in which the primary coolant was lost before the 0.5-hour fire ended. Figure 20 shows how the temperatures in the cask vary within the first hour after loss of coolant. The temperatures as a function of time, up to 40 hours after loss of coolant, are presented in Figure 21. Figure 22 displays the temperature profile in the cask at the arbitrarily selected cut-off point of 40 hours.

The IF-300 spent fuel shipping cask shown in Figure 1 carries seven fuel assemblies of the type shown in Figure 2. An evaluation of the fission gas

FIGURE 20. Temperatures in the IF-300 Following Loss of Coolant (0 to 1 Hour After Loss of Coolant)

FIGURE 21. Temperatures in the IF-300 Following Loss of Coolant (0 to 40 Hours After Loss of Coolant)

FIGURE 22. Temperatures in the IF-300 40 Hours After Loss of Coolant

release from this cask was made assuming that these seven fuel assemblies were the Design Basis PWR 1 fuel assemblies described in Tables 1 and 2. The calculated fission gas inventory and activity for this spent fuel after 90 days cooling time were obtained from Reference 1 and are presented in the Appendix in Table 3-1. To be conservative, General Electric assumed a 90 day cooling period instead of the design basis 120 days. This same conservative cooling time was used in the present study.

In the early stages of this study, the most severe situation conceivable was simulated first to determine the sequence of events that might lead to fission product release. The most severe situation envisioned was the immediate loss of primary coolant at impact, along with loss of the solar shield, loss of the water in the outer jacket, and immersion in a fire at 1475°F. Calculations were made for fires of 0.5 and 2.0 hours duration. In this initial phase of the study, a conceptual design of an LWR-type cask with a lead shield was simulated. The results of these early calculations showed that the length of the fire had little effect on the behavior of the cask internals during the fire, but there was an important effect on the fate of the lead shield. It was found that none of the lead melted during the 0.5-hour fire, but that the outer 1.0 inch, representing about 14% of the total volume of the lead shield, melted away at about 1.33 hours into the 2.0-hour fire. For this type of cask design, the loss of this amount of lead would have two consequences: (1) it would reduce the amount of radiation shielding, and (2) it would result in higher temperatures of the cask internals because the resulting gap would present a barrier to the heat attempting to flow to the cask surface. These higher temperatures, in turn, would result in higher pressures in the pin voids and a more rapid release of fission gases.

Simulation of the behavior of the AMCO cask following emptying or loss of its primary coolant gave results indicating that the fuel in this cask might not release any of its fission products, at least not by 52 hours after the coolant is lost. At this time, the temperatures in the cask appear to be approaching a new steady-state distribution (see Figure 23). The temperature of the hottest fuel pins is about 1397°F, but the corresponding pressure in the pins is 500 psia, compared to a pressure of about 990 psia required

FIGURE 23. Temperatures in the AMCO Cask Following Loss of Coolant

to burst the pin clads. There are two factors that might explain why the fuel pins in the IF-300 burst while those in the AMCO cask do not:

1. The internal pressure in the LMFBR fuel pins at 1397°F is 500 psia, while the internal pressure in the fuel pins in the IF-300 would be about 5 times as much at about the same temperature. The fuel pin pressures for the IF-300 were calculated using the procedure outlined on pages 9-11 of Reference 1 and on pages 150-151 of Reference 7. The fuel pin pressures for the AMCO cask were calculated using a slightly different approach, but were based on an end-of-life pressure in the pins of 750 psia at 1100°F, assuming 100% of the fission gases were released from the fuel. Details of the two approaches are presented in the Appendix in Section 3.2.1. The stresses in the clads of the fuel pins in the IF-300 model were determined from an equation relating the hoop stress to the pressure differential across the clad wall (see Section 3.2.1 of the Appendix). The stresses in the fuel pin clads in the AMCO cask were not calculated directly by the simulation model. Instead, experimental data on burst pressures as a function of temperature for Type 316 stainless steel clads were programmed into the model to monitor clad failure. The clad stresses were calculated later from pressures obtained from the model. The validity of this procedure was partially confirmed as described below. Since the hoop stress is proportional to the pressure differential across the clad wall, the ratio of a calculated stress to the allowable stress (100 hours creep rupture) at 1000°F was compared to the corresponding ratio of pressure differentials. The ratios were the same. The differential pressure corresponding to the allowable stress was the difference between the burst pressure at the same temperature, and the cask cavity pressure (see Section 3.2.1 of the Appendix).

2. The decay heat rate used in the simulation model of the IF-300 was 76.8 kw (262,000 B/hr), while that used in the simulation model of the AMCO cask was 19.8 kw (67,577 B/hr). The total heat load on the IF-300 was about 3.9 times that on the AMCO cask.
3. The outer surface of the AMCO cask is normally cooled by water contained in a 4-inch jacket partitioned by circumferential cooling fins, attached to the outer surface of the cask wall, which extend through the jacket and protrude 8 inches beyond the outer surface of the jacket. The outer surface of the IF-300 is also normally cooled by water contained in a 6-inch jacket, except that there are no cooling fins extending through and beyond the outer surface of the jacket. The outer surface of the IF-300 jacket is a corrugated barrel, where the corrugations provide some of the advantages of a finned surface. When the outer jacket is ruptured in an accident and the jacket water is lost, the fins on the AMCO cask allow heat to be conducted from the cask surface, through the empty water jacket, to the outer surface of the cask where it is dissipated by natural convection and radiation to the surroundings. In contrast, the empty water jacket on the IF-300 represents a substantial barrier to heat flow since, in the absence of fins, heat must be transferred through the jacket to the outer corrugated barrel by natural convection and radiation. This results in higher temperatures in the cask.

The AMCO spent fuel shipping cask shown in Figure 3 carries nine fuel assemblies of the type shown in Figure 4. It was assumed that these nine fuel assemblies were average assemblies, i.e., each had been operating in the reactor at an average power of 5.2 MW. The calculated fission gas inventory and activity for this spent fuel after 120 days cooling time were derived from results presented in Reference 12 for fuel assemblies that had been operating at 7.0 MW each. These data are presented in Tables 3-4 and 3-5 in the Appendix.

A model was developed for both the IF-300 and the AMCO cask to simulate the transient behavior of volatile solids or solid fission products (cesium compounds) that may be released as an aerosol from the fuel pins to the cask containment at the time the pins burst and the fission gases are released. This model was based on the basic coagulation equation for aerosols having a distribution of particle sizes, modified to include terms for particle removal or loss to the system and a source term.⁽¹¹⁾ The coagulation equation was further modified by eliminating the agglomeration terms by using a "self-preserving" particle size distribution function.⁽¹²⁾ A coagulation equation or particle balance equation was written for each of five particle size groups. Each of these particle balance equations was reduced to source, removal and storage terms by using the self-preserving particle size distribution function to determine the number of particles in each size group at any instant of time. Actually, this is mathematically factored into the particle balances through the settling, plateout and source terms (see Section 4 in the Appendix). A stirred settling rate equation and a plateout equation (based on a diffusional process) were obtained from the work of R. J. Davis.⁽¹²⁾ The source term used is a pulsed input term representing the release of particles from the bursting fuel pins. The particles in the source term are distributed according to the self-preserving size distribution function. The storage term, when integrated over time, gives the number of particles suspended in the cask containment in five arbitrarily selected particle size groups. These five particle size groups encompass particle radii ranging from a minimum of 0.08 microns to a maximum of 0.7 microns. The smallest radius is apparently characteristic of the minimum or so-called primary particle size, based on observation of stainless steel-UO₂ aerosols.⁽¹²⁾ The largest radius is apparently characteristic of the maximum particle size for chain agglomerates, as observed for steel oxide agglomerates.⁽¹²⁾ Further work is planned to determine the correct particle size range either from first principles or from later experimental data that might be available. Details of the development of the aerosol model are presented in Section 4 in the Appendix.

Of all the potentially volatile solids in PWR fuel, there is more cesium present than all the others combined. This cesium is not present as the metal, but probably exists as various chemical compounds including several oxides, the molybdenate, the iodide, the uranate and diuranate, and the zirconate. It was assumed that, when the pins burst, particles of these compounds would be released with the fission gases. Since the relative amounts of the compounds present are unknown, it was convenient to assume that they could all be considered to be the oxide Cs_2O .

Experimental data show that it is unlikely that more than 1% of the total cesium in all fuel pins will migrate to the pin void spaces during reactor operation, and of this amount less than 1% would be released under conditions postulated to occur in a severe transportation accident. The total cesium in the spent fuel in the IF-300 was calculated to be about 9300 grams, which is equivalent to about 1.13×10^6 curies. Therefore, only about 0.01% of this amount, or about 113 curies, would be released when the clads burst. General Electric's analysis of the release of fission products from the spent fuel in the IF-300 ⁽¹⁾ was limited to the release of the fission gases I, Kr, and Xe. Consequently, the fission product inventories presented in Reference 1 did not include cesium. The above estimates of the amounts of cesium present in the spent PWR fuel were derived from fission product inventories for spent Diablo Canyon reference fuel that had been cooled 90 days. ⁽¹⁴⁾ A small correction factor was applied to these data to account for differences in exposure.

The radioactivity in the solids suspended in the aerosol in the IF-300 containment, as a function of time after the accident, is presented in Figures 24 and 25. The peak values coincide with the times the fuel pins burst in each of the seven fuel nodes (the pins in some of the nodes burst simultaneously). Figures 24 and 25 show that about 47% of the particles (equivalent to about 53 curies) settle or plate out within 24 hours after the accident. At 24 hours, the activity of the particles still in suspension is only about 60 curies. The particles still in suspension at this time

FIGURE 24. Total Radioactivity in Volatile Solids Suspended as an Aerosol in the IF-300 (Breach Up Position, Breach Areas 0.025 and 0.25 Sq. Inches)

FIGURE 25. Total Radioactivity in Volatile Solids Suspended as an Aerosol in the IF-300 (Breach Down Position, Breach Areas 0.025 and 0.25 Sq. Inches)

are the smallest particles, those in a size range from 0.08 to 0.2 micron (an average of 0.11 micron) and those in a size range from 0.2 to 0.33 micron (an average of 0.25 micron).

At present, the model does not include a subterm of the removal term to account for leakage of aerosol from the cask containment through the damaged pressure relief valve. However, a system of equations has been developed to define the rate of flow of fission gases and particles from a cask. These equations were developed too late to be included in the present sets of models, but they may be included in the appropriate models during a later development phase. Most of the equations in this system will become part of the loss-of-coolant models and will form the basis for the leakage term in the volatile solids release models. The development of these equations is presented in Sections 3.5 and 4.1.5 in the Appendix, along with suggested procedures for their inclusion in the models.

The leakage term is expected to be greater than both the settling and plateout terms. This will alter the results of the analysis, as typified by Figures 24 and 25, significantly. A large leakage term would increase the rate of removal of aerosol from the cask. This means that those portions of the plots in Figures 24 and 25 that represent decreasing radioactivity in the cask, due to removal of particles by settling and plateout, would now have steeper slopes because of the more rapid rate of removal from the cask containment due to leakage. The magnitude of the leakage term is not known at this time.

If the cask is designed with a filter between the cavity and the relief valve, some of the particles in the aerosol might be removed before the aerosol reaches the surroundings. This filter would have to be independent of the relief valve and located at a point where it would not be damaged, even if the relief valve is sheared off. The volatile solids release model, especially the leakage term, would be useful in evaluating possible filtering media or devices.

The release of fission gases and solid fission products reported here represent only the free gases and solids present in the pin voids. Earlier in the study, another mechanism of release was considered that resulted in the release of the remaining "bound up" gases and solids. This mechanism was the oxidation of UO_2 to U_3O_8 , a fine granular material, from which these bound up gases and solids could more easily be released. As the study progressed, however, this mechanism appeared less and less likely. This was apparent from the results of the chain of simulations that seemed to indicate that the cask would be at a pressure higher than its surroundings. This would prevent influx of air to the fuel containment vessel.

There are at least two factors tending to make the pressure inside the cask higher than its surroundings. First, residual coolant vapor may be present in the cask for some time following the loss of primary coolant. The pressure of this residual vapor would increase as the vapor is heated, which should keep the pressure higher than atmospheric. Second, the fission gases are released from the fuel pins at a pressure high enough to burst the clads. For the IF-300, this pressure is about 1896 psia, which corresponds to a fuel pin temperature of about 921°F. This would be the driving force that would propel the fission gases, along with the cesium compounds, from the pins as an aerosol. This release of fission gases would tend to prevent outside air from entering the cask. Without this air, oxidation of the exposed fuel would be quite unlikely. Although the pressure would drop considerably as the gases expand into the cask containment, it might increase again by some small amount as the gases are heated by the fuel assemblies.

Oxidation of the fuel by the water vapor in the IF-300 has not yet been evaluated, but it is not expected to be significant.

D. Event Network

The event network of Figure 26 was constructed after the events and their relative times of occurrence were obtained using the simulation models developed for the IF-300 and AMCO casks. The network originates with the initial event "impact", and terminates with the following nine events:

HEDL 7507-30.46

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
(Page 1 of 10)

HEDL 7507-30.47

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
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HEDL 7507-30.48

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
(Page 3 of 10)

HEDL 7507-30.49

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
(Page 4 of 10)

HEDL 7507-30.50

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
(Page 5 of 10)

HEDL 7507-30.51

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
(Page 6 of 10)

HEDL 7507-30.52

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
(Page 7 of 10)

HEDL 7507-30.53

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
(Page 8 of 10)

HEDL 7507-30.54

FIGURE 26. Network of Events Following a Spent Fuel Shipping Cask Accident
(Page 9 of 10)

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1. Radiation leakage
2. No radiation leakage
3. New steady-state condition reached
4. New or original steady-state condition reached
5. Solid and soluble fission products released from cask
6. Volatile solids escape from cask
7. Volatile solids do not escape from cask
8. Fission gases escape from cask
9. Fission gases do not escape from cask.

Two of the event blocks or nodes of the network represent conditions rather than events. These conditions are "LWR-type cask" and "LMFBR-type cask."

A choice of a path through the network is allowed by the branching paths emanating from some of the events, and by the logic gates "AND", "INCLUSIVE OR", and "EXCLUSIVE OR". This type of event network combines the decision or event tree construction with the logic gates of a fault tree. The logic gates focus or fold the expanding branches of the event tree.

The accented lines connecting some of the events in the network of Figure 26 represent paths revealed by use of the simulation models discussed in this report, in their present stage of development. It is apparent that several paths have not been investigated.

Eventually, probabilities and times will be determined for the paths connecting the events. These calculated probabilities and times will be obtained from parametric studies using the simulation models. Network algebra will be used to calculate the most probable path to the terminal events, and the probability of each of the terminal events, considering all the possible paths. Because of its size and complexity, the event network will be evaluated using the computer code GERT⁽³⁰⁾ developed for this purpose.

The cask accident event network may be imbedded, as a subnetwork, in a larger, more comprehensive event network for the entire shipping study.

Figure 26 identifies the events that may lead to a release of fission gases. Measures taken to prevent or delay these events could form a strategy of "defense in depth" for cask designers. The Cask Designer's Guide⁽⁷⁾ does not identify levels of safety for shipping casks per se, but does discuss the integrity of cask containment following impact, including the protection of closures from impact (valves, pressure relief lines, etc.), energy absorbers, and the integrity of the cask's seal. It may be useful to attempt to identify "levels of safety" for cask design that would serve a function similar to the three levels of safety identified for nuclear reactors.⁽⁶⁾

Figure 26 identifies the events that may lead to a release of fission gases. Measures taken to prevent or delay these events could form a strategy of "defense in depth" for cask designers. The Cask Designer's Guide⁽⁷⁾ does not identify levels of safety for shipping casks per se, but does discuss the integrity of cask containment following impact, including the protection of closures from impact (valves, pressure relief lines, etc.), energy absorbers, and the integrity of the cask's seal. It may be useful to attempt to identify "levels of safety" for cask design that would serve a function similar to the three levels of safety identified for nuclear reactors.⁽⁶⁾

CONCLUSIONS AND RECOMMENDATIONS

The IF-300 loses its primary coolant at a much faster rate than the AMCO cask following an accident in which a breach is opened in the cask containment. The breach is assumed to be due to a relief valve, which is either sheared off or stuck in a partially open position due to damage at impact. Breach flow areas in these cases were assumed to be 0.25 in^2 and 0.025 in^2 , respectively. Results of the simulations show that, for the largest breach flow area and with the casks in a breach down position, it takes about 15 minutes to empty the IF-300 of its primary coolant and about 43 minutes to empty the AMCO cask. Since the accident conditions include a 30-minute fire, it is obvious that, in this case, the casks could not be approached to take measures to prevent the loss of the coolant. For the smallest breach flow area, with the casks in the same breach down position, the IF-300 loses its coolant in about 1.5 hours while the AMCO cask loses its coolant in about 7.0 hours. It is not likely that loss of the coolant from the IF-300 in this case could be prevented since, during the 30-minute fire, about 22% of the coolant is lost, and the rest would be lost before the cask cooled enough to be approached. In the case of the AMCO cask, however, enough time might be available to take some remedial steps to prevent the loss of a substantial portion of the coolant. For the largest breach flow area and with the casks in a breach up position, it takes about 66 minutes to empty the IF-300 and about 20 days to empty the AMCO cask. For the smallest breach flow area and with the casks in a breach up position, it takes about 4.18 hours to empty the IF-300 and about 20 days to empty the AMCO cask. It is not likely that much could be done to prevent the loss of coolant from the IF-300, but it appears that ample time would be available to prevent the loss of coolant from the AMCO cask.

The differences in the coolant loss rates are due to the vapor pressures of the different coolants at the time of the accident. The average temperature of the water in the IF-300 during normal operating conditions was determined to be about 347°F , while that of the Dowtherm-A in the AMCO cask was determined to be about 360°F . The saturation pressure of water at 347°F is 130 psia. The saturation pressure of Dowtherm-A at 360°F is 2.0 psia, far below atmospheric pressure, which means that this coolant is subcooled.

When a breach is opened in the IF-300, water will be driven through the opening mainly due to the high pressure in the cask. If the cask is in a breach down position, saturated liquid will be expelled and, if the cask is in a breach up position, saturated vapor will be expelled.

When a breach is opened in the AMCO cask, the Dowtherm-A will be driven through the opening due to forces other than the internal pressure in the cask. The internal pressure in the cask would probably be near atmospheric pressure, so this driving force would not be a factor. If this cask is in a breach down position, the Dowtherm-A would be driven through the opening due to the force exerted by the liquid column. If the cask is in a breach up position, the Dowtherm-A would leave the cask as a vapor. However, in this case, the Dowtherm-A is subcooled and must wait until enough heat is absorbed to bring its temperature to 494.8°F, its saturation temperature at atmospheric pressure. Also, at night, heat transfer from the Dowtherm-A-cooled cask to the surroundings improves with the removal of the solar heat input. This reduces boil-off since less heat is available to the coolant.

It is apparent that casks using coolants with low vapor pressures would have substantially lower coolant loss rates. As a result, more time would be available to prevent the loss of the coolant and to take steps to restore the cask to near normal operating conditions.

As discussed earlier, results of the simulations would indicate that there would not be enough time to prevent the loss of coolant from the IF-300, but that enough time might be available to prevent the loss of coolant from the AMCO cask and to restore it to near normal operating conditions. A simple, but effective, procedure would be to bring the cask to a breach up position (if it is not already in this position), replace the solar shield, and reintroduce water into the outer jacket. Once these measures are taken, then attention could be focused on ways to close the breach.

The fuel pins that fail first in the IF-300 burst at about 4 hours following the accident when the cask is in the breach down position and the breach flow area is 0.025 in^2 . It is the smallest time span of the

four cases considered. All of the coolant is lost in about 2 hours, and the first fuel pins burst 2 hours later. If the cask cools sufficiently and other conditions permit, the following are suggested as possible steps that might prevent or delay overheating and bursting of the pins. Introduction of an inert gas to the cask cavity might provide enough cooling to prevent bursting of the pins. Air is to be avoided to prevent oxidation of the fuel if the cooling attempts fail. Also, water is to be avoided since it would probably flash to steam, which might force radioactive particles from the cask. If it were possible, the introduction of small-diameter steel shot, along with the inert gas, would provide an additional heat sink capability. Also, the shot, with the gas in the voids, would provide a good conduction path from the fuel to the cask wall. At the same time, water could be introduced into the water jacket at the outer surface. It is recommended that the effectiveness of these measures be evaluated in later studies.

An analysis of the behavior of the AMCO cask following loss of its primary coolant produced results that indicate the pins in this cask might not burst and, consequently, no fission products would be released. This might be due to any one of the following three factors, or a combination of all three. First, the internal pressures in the fuel pins are about half that required to burst the pins, even at 52 hours after the primary coolant is lost. Second, the decay heat rate of the spent fuel in this cask is about one-fourth that of the spent fuel in the IF-300. Finally, the AMCO cask, unlike the IF-300, has circumferential cooling fins attached to the outer surface of the cask wall, extending through the water jacket and protruding 8 inches beyond the outer diameter of the cask. When the water in the outer jacket is lost at the time of the accident, these fins continue to provide a path for heat flow. Without these fins, the heat would have to be transferred across the empty water jacket by natural convection and radiation and, as a result, the temperatures in the cask would be higher. It is recommended that, if a cask is designed with a water jacket as a neutron shield, cooling fins extending through the jacket should be included as part of the design. It is also recommended that, in subsequent phases of this study, the calculation of internal pressures in the fuel pins and

the validity of the burst pressure data be reviewed to verify the results obtained.

As stated earlier, in the Results and Discussion section, some of the fuel pin clads may be damaged at impact. The extent of this damage could be estimated using mathematical models based on experience gained in setting up similar models in the past. It is recommended that these models be developed.

Results from the simulation of the behavior of the IF-300 following loss of its primary coolant indicated that all of the fuel pins in this cask would burst, releasing about 11,900 curies of fission gases (about 33% of the total in the spent fuel) and about 113 curies of fission product solids, assumed to be Cs_2O (representing about 0.01% of the total cesium in the spent fuel). A model simulating the behavior of the aerosol formed by the fission gases and the Cs_2O particles showed that, if the aerosol were confined to the cask cavity, about 47% of the particles (about 53 curies) would settle or plate out within 24 hours after the accident. The remaining 53% (about 60 curies) are suspended in the cask as an aerosol at this time. The particles suspended are those in two of the five size groups considered. These two size groups contain the smallest particles, those in the size range from 0.08 to 0.2 micron (an average of 0.11 micron) and those in the size range from 0.2 to 0.33 micron (an average of 0.25 micron). It is not known at this time how much of the aerosol would escape from the cask through the damaged relief valve. Equations have been developed to define the rate of flow of the aerosol from an opening in a cask's containment system; however, the equations were developed too late to be included in the sets of models discussed in this report. These equations will become part of the loss-of-coolant models and will form the basis for the leakage term in the volatile solids release models. It is recommended that these models be modified to include the equations describing the flow of fission products from the cask containment (see Sections 3.5 and 4.1.5 of the Appendix). The modified models would be used to determine the amount of fission products lost from a cask through a given breach flow area.

If a cask is designed with a filter between the cavity and the pressure relief valve, some of the solids in the aerosol could be removed before the

aerosol reaches the surroundings. The volatile solids release models, especially the leakage term, would be useful in evaluating possible filtering media or devices.

The amounts of fission gases and solid fission products reported here represent only the amounts present in the pin voids. In the early stages of this study, before the coolant loss rate models were developed, another mechanism of release was considered that resulted in the release of the remaining "bound up" gases and solids. This mechanism was the oxidation of the UO_2 to U_3O_8 , a fine granular material, from which these bound up gases and solids are more readily released. As the study progressed and the coolant loss rate models were developed, this mechanism appeared less and less likely. This was apparent from the results obtained from these models, which seemed to indicate that a cask would be at a pressure higher than its surroundings. This would prevent the influx of air, which is necessary for oxidation of the fuel, to the containment vessel.

In the very early stages of this study, the most severe situation envisioned was simulated first to give a preliminary "worst case" estimate of the extent of fission product release. The most severe situation envisioned was the immediate loss of primary coolant at impact, along with loss of the solar shield, loss of water in the outer jacket, and immersion in a fire at 1475°F. Calculations were made for fires of 0.5 and 2.0-hours duration. The cask modeled in this initial phase of the study was neither the IF-300 nor the AMCO cask. It was an early conceptual design of an LWR spent fuel shipping cask with lead shielding. The results of the calculations showed that the length of the fire had little effect on the thermal behavior of the cask internals, but there was an important effect on the fate of the lead shield. It was found that none of the lead melted during the 0.5-hour fire, but that the outer 1.0 inch, representing about 14% of the lead shield, melted away at about 1.33 hours into the 2.0-hour fire. The loss of this much of the lead shield would have two consequences:

- (1) It would reduce the amount of radiation shielding, and
- (2) It would result in higher temperatures of the cask internals because the resulting gap would present a barrier to the heat flowing to the cask surface. These higher temperatures would, in turn, result in higher pressures in the fuel pins and a more rapid release of fission products.

In summary, the results of the simulations for the accident conditions considered indicate that the IF-300 would lose its primary coolant at a much faster rate than the AMCO cask and that, after the coolant is lost, all of the pins in the IF-300 would burst, releasing all the fission gases (11,900 curies) and a small percentage of cesium (113 curies) from the pin voids. In contrast, the fuel pins in the AMCO cask do not burst and no fission products are released from the voids. Several factors were cited to explain the difference in performance:

- (1) The different coolant loss rates are due to the vapor pressures of the different coolants used. The IF-300 uses water which, at the time of the accident, has a vapor pressure about 9 times atmospheric. The AMCO cask uses Dowtherm-A, which is subcooled at the time of the accident.
- (2) Long after loss of primary coolant (52 hours), the pressures in the fuel pins in the AMCO cask are only about half that required to burst the pins. In contrast, all the fuel pins in the IF-300 burst between 7 and 13 hours after loss of its coolant, depending upon breach size and cask orientation. (This could be the result of a number of other related factors, including pin design and the factors listed below).
- (3) The decay heat rate of the spent fuel in the AMCO cask is about one-fourth that of the spent fuel in the IF-300.
- (4) The AMCO cask, unlike the IF-300, has cooling fins attached to the outer surface of the cask wall extending through the water jacket. These fins provide a path for heat transfer even when the jacket water is lost.

APPENDIX

The objectives of this study have been to develop simulation models of typical casks for the rail shipment of spent fuel from nuclear reactors, to use these models to study the behavior of the casks following a postulated accident and fire, and to determine the extent of radioactive releases from the casks following the accident. The casks modeled were the IF-300, designed by General Electric for the shipment of spent LWR fuel ⁽¹⁾, and a cask designed by the Aerojet Manufacturing Company (AMCO) for the shipment of spent LMFBR fuel. ⁽²⁾

This study has progressed by definite steps or stages, with each successive stage being an improvement or refinement of the total modeling effort. These improvements or refinements were based on what had been learned from the preceding stages, and on new information gathered from other sources. An attempt will be made in these opening paragraphs of the Appendix to outline, in chronological order, some of the more important stages of this "bootstrapping" process.

At the outset, it should be made clear that the IF-300 was not modeled until the final stages of the study. The LWR spent fuel shipping cask modeled and studied through most of the study was a conceptual design that was never actually built. There are several important differences between the IF-300 and this conceptual design. First of all, lead was used for the gamma shield in the conceptual design instead of depleted uranium. Second, the neutron shield or outer water jacket of the conceptual design is partitioned by circumferential cooling fins attached to the outer surface of the cask wall, extending through the jacket and protruding several inches beyond the outer surface of the water jacket. Although this same type of fin structure was used in the AMCO cask, the IF-300 design does not include fins. Instead, the IF-300 uses a corrugated shell as the outer surface of the water jacket, where the corrugations offer some of the advantages of fins. However, if the outer jacket loses its water, it would become a substantial barrier to heat flow from the cask, since no fins extend through the jacket to the cask wall. Third, the corrugated outer surface of the water jacket on the IF-300 is cooled by air forced over the surface by diesel-driven blowers. The conceptual design relies on air flowing over

the fins by natural convection, along with radiant heat transfer, to cool the outer surface. Finally, the conceptual design uses thick, massive baskets to contain the fuel assemblies. These baskets are made of sandwiched layers of copper and boron carbide for criticality control. Both copper and boron carbide have high thermal capacities that make these baskets potentially effective heat sinks. By contrast, the IF-300 uses thin slotted stainless steel baskets with B_4C -filled stainless steel tubes welded to the baskets for criticality control.

Some statements made in the Introduction to summarize the modeling effort will be repeated to provide some orientation before launching into the chronological account of the study and detailed discussions of the models.

A set of five simulation models has been developed for the IF-300, and a set of similar models for the AMCO cask. These models simulate cask behavior during normal operating conditions, and during conditions following an accident and fire. The sets of models include:

1. A model simulating the steady-state thermal behavior of a cask prior to an accident.
2. A model that determines the transient thermodynamic behavior of a cask and the gradual loss of primary coolant following impact and opening of a breach in the cask containment. This model applies to the case where the cask comes to rest with the breach down.
3. A model simulating the transient thermodynamic behavior of a cask and gradual loss of primary coolant following impact and opening of a breach in the cask containment. This model applies to the case where the cask comes to rest with the breach up.

4. A model simulating the transient thermal behavior of a cask following the eventual loss of primary coolant.
5. A model simulating the transient behavior of the volatile solids or solid fission products (cesium compounds) that may be released to the cask containment as an aerosol at the time the fuel pins burst and the fission gases are released.

Of these models, the second, third and fifth were developed for programming on MIMIC, a continuous system simulation program.⁽³⁾ The first and fourth models were programmed on the TAP simulation code, a network analyzer.⁽⁴⁾ For the IF-300, portions of the second and third models are represented by a chart devised by Moody⁽⁹⁾ that relates the maximum steam and water flow rates to the local stagnation properties in a pressurized vessel. For the AMCO cask, the second model is an energy balance that relates the potential energy of the coolant column to the mass velocity of the coolant flowing from the breach and the time required to empty the cask.

Figure A-1 shows the information flow between models and the order in which they are used.

Radioactivity could be released from the casks as fission products if the primary coolant containment is breached. In this study, the fission products are the fission gases and volatile solids or solid fission products (cesium compounds) in the spent fuel. In addition to the sets of models listed above, equations were developed to define the rate of flow of these fission products from the casks. These equations were developed too late to be included in the sets of models. However, they will be included in the appropriate models during a later development phase. The derivation of these equations is discussed here, along with discussions of the development of the models.

At the time the study of spent fuel shipping cask accident behavior was begun, it was decided to start with the most pessimistic case to determine at the outset the most conservative estimate of fission product release and the times of release. The most pessimistic case visualized was one in which a cask loses its solar shield, outer jacket water, and primary coolant at

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FIGURE A-1. Information Flow Among Simulation Models

the instant an accident occurs, and it is subjected to a fire at 1475°F for at least 0.5 hour. Consequently, the first simulation models constructed were so-called "loss-of-coolant" models.

To provide initial conditions for the loss-of-coolant models, a steady-state pre-accident version of each of the models was constructed in which use was made of the concept of volumetric heat dissipation to represent heat transfer from the fuel regions to the coolant. In these steady-state models, of course, the solar shield remained intact and the outer jacket was water-filled.

As the study progressed, the emphasis shifted from simulation of the pessimistic to an effort to approach realism. The first step in this direction was prompted by the desire to relax what was thought to be the rather severe assumption that all of the primary coolant is lost instantaneously at the moment of impact. This led to the development of what will be referred to as the "no-loss-of-coolant" models. These models were eventually to become the "coolant loss rate" models but, at first, they were developed to study cask behavior following an accident and fire with no loss of primary coolant. It was assumed that the only damage sustained by the casks was loss of their solar shields and the water in the outer jackets, and that the pressure relief system was inoperable. The temperatures obtained from these models approached new, higher steady-state values. This presented no problem in the case of the AMCO cask since its primary coolant is Dowtherm-A, a coolant with a vapor pressure about equal to that of atmospheric pressure at its new steady-state temperature. However, since the primary coolant in the conceptual LWR cask design considered is water, its internal pressure reached an intolerable level.

Later, the no-loss-of-coolant models were modified to form the "coolant loss rate" models. These new models were designed primarily to estimate the rate at which primary coolant would be lost from the casks following impact and opening of a breach in the cask containment. They also simulated the transient thermodynamic behavior of the casks following these events, during a fire, and while the coolant was being lost from the cask.

It was difficult to conceive of an accident situation severe enough to cause a breach in the primary coolant containment, since these casks are extremely well designed. Also, results from various experimental programs, including 30-foot drop tests, puncture tests, etc., in which cask models were used, indicated that the chances of a cask containment being breached in this manner would be extremely small, in fact, quite unlikely. It seemed reasonable to assume, however, that any access to the primary coolant that had been included as part of the cask design, such as pressure relief passages and valves, fill passages and valves, etc., might be vulnerable to damage or malfunction. Since the function of the pressure relief valve is to automatically respond to changes in conditions that may occur in the coolant-filled cask cavity, it seemed reasonable to assume that this would be the most vulnerable access to the coolant and the most likely candidate for a breach-causing failure. Although this valve is usually well protected, it was assumed that it could be jarred sufficiently at impact to be forced into a partially open position, or it could fail to reseal after performing its function during normal operating conditions. To arrive at an upper limit to the damage that might occur to this valve at impact, it was assumed that it could be sheared off entirely, resulting in more than a full open position.

About the time the development of the coolant loss rate models was nearing completion, work had begun on a simulation model to determine the behavior of volatile solids released as an aerosol from the fuel in the casks following loss of primary coolant. At first, this model was incorporated into the loss-of-coolant models, but this proved to be cumbersome, so a separate model was developed.

Finally, the second step to approach realism or "real world" conditions was taken in the final stages of the study when the conceptual design of an LWR spent fuel shipping cask was replaced by the "real" IF-300. All of the LWR cask models were restructured to simulate the IF-300.

This account of the order in which the models were developed sets the stage for more detailed discussions of each of the models. The models are linked together and used in a sequence quite different from the order of

their development (see Figure A-1). The discussions that follow are in the order of each model's use in the chain of Figure A-1, rather than in the order of their development. For this reason, in some of the sections, some references may be made to equations derived in subsequent sections. In some cases, the derivation of certain equations and concepts may be included in an earlier section where they may be presented in a more logical order, even though they were first derived for a model in a later section.

1. CASK SIMULATION MODELS FOR STEADY-STATE CONDITIONS PRECEDING THE ACCIDENT

The models discussed in this section are referred to as "Steady-State Pre-accident Simulation Models." These models were developed first to provide the initial conditions for the post-accident transient analyses. They simulate conditions in the casks while in transit, during an uneventful, normal trip. Later, modifications to these models produced the so-called "Loss-of-Coolant" models discussed in Section 3. Both the pre-accident and loss-of-coolant models are programmed on the TAP Simulation Code.⁽⁴⁾

Before the steady-state models are discussed, the IF-300 and AMCO casks will be described. The steady-state models will then be discussed and compared to the loss-of-coolant models. Following this, in Section 1.1, the coolant circulation patterns and heat transfer paths in the casks will be discussed, and, in Sections 1.2 and 1.3, equations will be derived that define some concepts used in the development of the models.

The IF-300 carries seven PWR fuel assemblies (see Figures 1 and 2). These assemblies are surrounded by slotted stainless steel baskets. Several B_4C -filled stainless steel tubes are attached to the outer surfaces of the baskets for criticality control (see Figure 3). The seven assemblies and their baskets are contained in an inner cavity filled with water. This fuel containment cavity is surrounded by 4 inches of depleted uranium encased in stainless steel. The outer surface of the uranium is cooled by water contained in a 6-inch jacket. The type of fuel assembly carried by this cask is shown in Figure 4, and detailed data are presented in Table 2.

The AMCO cask simulated is shown in Figure 5. This cask carries nine fuel assemblies of hexagonal cross-section, each encased in a steel basket with slots for crosswise coolant flow. The nine assemblies and their baskets are contained in a stainless steel canister filled with either Dowtherm-A or sodium. The cask analyzed in this study was assumed to be filled with Dowtherm-A. The fuel assemblies are arranged in a circular pattern, bounded on the inside by a coolant expansion chamber of 15.5 inches diameter, and bounded on the outside by the inner wall of the containment vessel or canister. The canister has a

one-inch thick wall that is separated from the inner wall of the containment vessel by a 0.25-inch helium-filled gap. The containment vessel is surrounded by a 3.625-inch thick uranium shield which, in turn, is surrounded by a 6-inch thick steel shell. The outer surface of the steel shell is cooled by water contained in a 4-inch jacket partitioned by circumferential cooling fins, which extend through the jacket to protrude 8 inches beyond the outer diameter of the jacket. The fuel assembly carried by this cask is shown in Figure 6, and detailed data are presented in Table 4.

The coolant circulation pattern and heat transfer paths in the IF-300 are discussed in Section 1.1 and illustrated in Figures 1-1 and 1-3. A similar circulation pattern exists in the AMCO cask, but the heat transfer paths are somewhat different, as shown in Figure 1-2.

In both casks, the decay heat generated in a fuel assembly is transferred from the fuel pins to the primary coolant inside the fuel assembly can by natural convection. The coolant, in turn, transfers the heat to the inner wall of the fuel assembly can, also by natural convection. The heat is then conducted through the can wall and is transferred by natural convection to the primary coolant outside the fuel assembly cans, in the cask cavity. Most of the decay heat from the fuel pins is dissipated in this manner. A small amount is transferred radially through the fuel assembly by conduction, but this is negligible compared to that transferred by natural convection to the coolant and then to the can wall. In the IF-300, the heat in the cask cavity is transferred to the inner wall of the containment vessel by natural convection, and then by conduction through the steel shells and the uranium shielding, eventually arriving at the inner surface of the neutron shield or outer water jacket. In the AMCO cask, the heat in the cask cavity is transferred to the inner wall of the canister by natural convection, and then by conduction through the canister wall to the helium gap, by radiation and conduction across this gap to the cask wall, and then by conduction through the steel and uranium in the cask wall to the inner surface of the water-filled neutron shield. The AMCO cask (and the conceptual LWR cask) are designed with circumferential cooling fins attached to the outer surface of the cask wall that extend through the water jacket and protrude beyond the outer surface of the jacket. Part of the heat from

the cask wall is conducted through these fins, through the jacket, and is dissipated to the surroundings by natural convection and radiation from the fins. The rest of the heat is transferred to the water in the outer jacket by natural convection which, in turn, transfers the heat to the outer surface of the jacket (and to the fins) by natural convection, where it is then conducted through the jacket wall and finally dissipated to the surroundings by natural convection and radiation. The IF-300 does not have fins such as those just described. However, the outer surface of its water jacket is corrugated, and the corrugations provide some advantages of a finned surface. In addition, the IF-300 is cooled at the outer corrugated surface by air forced over the corrugations by diesel-driven blowers.

The steady-state model of the conceptual cask was constructed first, but was sufficiently general to be easily adapted to the IF-300 and AMCO casks. The primary difference between the LWR casks and the AMCO cask is in the layout of the fuel assemblies and baskets in the containment vessel.

An idealized model of the IF-300 is shown in Figures 3-1 and 3-2. The primary difference between this model and the actual cask is the representation of the fuel, fuel cans and baskets as circular regions rather than the array of square fuel assemblies. This simplified model was divided into radial nodes as shown in Figure 3-19. The network of admittances connecting these nodes is shown in Figures 1-1 and 3-20. An idealized representation of the IF-300 was necessary because the array of square fuel assemblies was not symmetrical (see Figures 2 and 3-2).

Unlike the IF-300, the arrangement of the fuel assemblies in the containment vessel of the AMCO cask is symmetrical. This allows the simulation network to be based on a symmetrical cut of the cask as shown in Figures 1-2 and 3-21. The hexagonal fuel assembly and its basket are represented as concentric cylinders divided into radial nodes as shown in Figures 3-3, 1-2 and 3-21. The baskets surrounding the fuel assemblies are designed with slotted holes for free passage of the coolant.

The steady-state models and the loss-of-coolant models are very similar. The primary difference between these models, of course, is that

the loss-of-coolant models are not steady-state models, but were developed to simulate transient conditions in the cask following an accident, fire, loss of solar shield, loss of coolant in the neutron shield, and eventual loss of primary coolant. This means that the simulation networks (electrical analogs) of the loss-of-coolant models include a thermal capacitance at all nodes representing material mass. Also, since the primary coolant and the coolant in the outer jacket were lost, except for some residual vapor, the convection admittances in the fuel assemblies, cask cavity, and in the outer jacket are for the vapor rather than the liquid. The conduction admittances in the fuel assemblies are also affected by the replacement of liquid by vapor. In addition, with the liquid coolant gone, admittances were added to the networks in the cavity and outer jacket to represent paths for heat transfer by radiation between surfaces. Loss of the solar shield required some additional changes at the outer surface of the cask.

Later, as the study progressed, circuits were added to the loss-of-coolant models to simulate melting of the lead shield (of the conceptual LWR cask), release of fission gases from the fuel pins due to bursting of the clads, and diffusion and oxidation of the fuel.

The simulation network for the steady-state pre-accident model of the IF-300 is presented as Figure 1-1, and the corresponding network for the AMCO cask is presented as Figure 1-2. These figures should be compared with Figures 3-19 and 3-20 for the transient loss-of-coolant model of the IF-300, and Figure 3-21 for the corresponding model of the AMCO cask.

A collection of fuel pins such as in the fuel assemblies have a "lumped" characteristic. A method was devised to "distribute" the "lumped" fuel to give homogeneous regions that could then be "re-lumped" to fit the nodal representation of the models. This was done by using the concepts of volumetric heat dissipation and an apparent thermal conductivity for materials with voids to represent the heat transfer in the fuel regions. The equations that define these concepts are presented in Sections 1.2 and 1.3, respectively. Equations that define the apparent thermal conductivity of a homogenized fuel region following loss of the primary coolant are derived in Section 3.1.

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FIGURE 1-1. Simulation Network of the Steady-State Model of the IF-300

FIGURE 1-2. Idealized Representation of the AMCO Spent Fuel Shipping Cask and Simulation Network of the Steady-State Model (Page 1 of 2)

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FIGURE 1-2. Idealized Representation of the AMCO Spent Fuel Shipping Cask and Simulation Network of the Steady-State Model (Page 2 of 2)

Equations representing heat balances on the various nodes are not presented here or in Section 3 since both the steady-state pre-accident models and the loss-of-coolant models are quite detailed, with many admittances and nodes, especially the loss-of-coolant models. Heat balances that are of the same form as those that could have been presented here are presented in Section 2 for the "coolant loss rate" models of the casks.

Listings of the simulation models programmed on the TAP code are not presented in this report since the format used is unique, and those not familiar with the code would find the listings of little value.

1.1 Coolant Circulation and Heat Transfer Paths in the Casks

In both casks, the decay heat generated in a fuel assembly is transferred from the fuel pins to the primary coolant inside the fuel assembly can by natural convection. The coolant, in turn, transfers the heat to the inner wall of the fuel assembly can, also by natural convection. The heat is then conducted through the can wall and is transferred by natural convection to the primary coolant outside the fuel assembly cans, in the cask cavity. Most of the decay heat from the fuel pins is dissipated in this manner. A small amount is transferred radially through the fuel assembly by conduction, but this is negligible compared to that transferred by natural convection to the coolant and then to the can wall. The heat in the primary coolant in the cask cavity is transferred to the inner wall of the containment vessel by natural convection.

An illustration of the complex coolant circulation pattern and the heat flow paths in the IF-300 (and conceptual cask) is presented in Figure 1-3. This figure represents a two-stage simplification process starting with the actual IF-300 layout showing the coolant circulation pattern, and ending with a network simulating the heat transfer from the fuel to the inner surface of the containment vessel wall. Figure 1-3(a) shows the actual cask layout and the coolant circulation pattern.

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FIGURE 1-3. Representation of Steady-State Cooling by Natural Convection in the IF-300 Before the Accident

The first stage of the simplification, shown in Figure 1-3(b), is based on the assumption that the square fuel assemblies can be represented by cylindrical assemblies, contained in a cylindrical can, and the canned assembly enclosed in a cylindrical slotted basket. It was assumed that the baskets in the coolant-filled steady-state pre-accident model would be at the same temperature as the coolant in the cavity, and that the simulation of the heat transfer in the cask cavity would not be affected if the baskets were neglected. This will not be the case in the loss-of-coolant models to be discussed later, where the baskets will definitely play a part in the transfer of heat by radiation. It was also assumed that the temperature drop across a can wall would be quite small, and that the can wall could be represented by a single node.

The coolant circulation flow pattern is shown in Figure 1-3(b), along with one of six 60-degree symmetrical segments of the cask containing typical heat transfer paths.

The final step of the simplification is shown in Figure 1-3(c). In this step, the assumption is made that there is no heat flow across the radial boundaries of the 60-degree segments, i.e., there is no heat flow angularly in the cask. This allows the fuel, cans, and coolant spaces to be represented as concentric rings. The heat transfer path shown is presented more clearly in Figure 1-3(d).

In Figure 1-3(d), four types of nodes are shown for the analog of the heat transfer paths: fuel nodes (F), can nodes (C), coolant nodes (W), and the node at the inner surface of the containment vessel wall (O). The arrows on the connectors between nodes point in the direction of heat flow. These heat transfer paths were described in the opening paragraph of this section.

The heat transfer paths in the AMCO cask are not as complex as those in the IF-300 since the basket arrangement is not as complex. In the AMCO cask, each fuel assembly and basket combination could be treated individually, rather than as concentric regions, since the cluster of nine fuel assemblies is symmetrical and no single assembly is located in the center of the cluster.

1.2 Volumetric Heat Dissipation

Simulation of the heat transfer from the fuel pins to the coolant in each fuel assembly required the use of a unique technique. Due to the complexity posed by the "lumped" nature of the fuel pin bundles, the concept of volumetric heat dissipation was used as a simplification.⁽¹⁵⁾ This concept, along with that of an apparent thermal conductivity, was used to "distribute" the "lumped" fuel to convert the fuel assemblies into homogeneous regions which could then be "re-lumped" into nodes for the heat transfer network. This concept was also used in the development of the coolant loss rate models of Section 2.

An energy balance on a differential volume element of this homogeneous or distributed fuel is illustrated in the following sketch:

An energy balance is usually written as

$$\text{Input-Output} = \text{Accumulation.} \quad (1-1)$$

The energy balance on the volume element is

$$q + Q_G - q - \frac{\partial q}{\partial r} \Delta r - Q_v = Q_s \quad (1-2)$$

where

- q = heat conduction, H/θ
- Q_G = heat generation, H/θ
- Q_V = heat dissipation, H/θ
- Q_S = energy accumulation or storage, H/θ .

The basic equation for heat conduction in this porous material is

$$q = - 2\pi r k_a \frac{\partial T}{\partial r} \Delta x$$

where

- k_a = an apparent thermal conductivity, $H/\theta LT$
- T = the temperature, T
- r = the radius, L
- x = the length of the element, L .

Differentiating this equation with respect to the radius gives

$$\begin{aligned} \frac{\partial q}{\partial r} &= - 2\pi r k_a \frac{\partial^2 T}{\partial r^2} \Delta x - 2\pi k_a \frac{\partial T}{\partial r} \Delta x \\ &= - 2\pi r k_a \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) \Delta x \\ &= - 2\pi r k_a \nabla^2 T \Delta x \quad . \end{aligned} \quad (1-3)$$

Heat generation in the element may be expressed as:

$$Q_G = 2\pi r q_G \Delta r \Delta x \quad (1-4)$$

where

- q_G = the volumetric heat generation in the porous material, $H/\theta L^3$.

Heat dissipation in the volume element is defined by the equation,

$$Q_V = 2\pi r H_V (T - T_0) \Delta r \Delta x \quad (1-5)$$

where

H_V = a volumetric heat dissipation coefficient, $H/\theta L^3 T$,

T_o = the coolant temperature, T .

Finally, the energy accumulation or storage in the volume element is

$$Q_s = 2\pi r \rho C \frac{\partial T}{\partial t} \Delta r \Delta x \quad (1-6)$$

where

ρ = the density of the porous material, M/L^3

C = the heat capacity, H/MT

t = time, θ .

Substituting from Equations (1-3), (1-4), (1-5) and (1-6) into Equation (1-2), and simplifying, the energy balance becomes

$$q_G + k_a \nabla^2 T - H_V (T - T_o) = \rho C \frac{\partial T}{\partial t} . \quad (1-7)$$

This equation is similar to that for heat transfer in a fin with heat generation, except that an apparent thermal conductivity is used for the porous material, and a volumetric heat dissipation coefficient is used instead of a conventional convection coefficient.

A fuel pin and its surrounding coolant was considered to be a "unit cell" as shown in the following sketch:

The surrounding coolant is represented by an equivalent cylinder rather than as the more complicated shape that would be traced by the common zero heat transfer boundary of adjacent pins.

The heat transfer from the pin to the coolant in the unit cell is

$$Q_v = 2\pi ah (T - T_o) \Delta x \quad (1-8)$$

where

Q_v = the heat transferred, H/θ

a = the fuel pin radius, L

Δx = the length of the unit cell, L

h = the heat transfer coefficient for natural convection from the pin to the coolant, H/θL²T

T = the average temperature of the fuel pin, T

T_o = the coolant temperature, T.

The heat transfer from the pin can be written in equivalent volumetric terms as

$$Q_v = \pi b^2 H_v (T - T_o) \Delta x \quad (1-9)$$

where

b = the radius of the unit cell, L

H_v = a volumetric heat dissipation coefficient, H/θL³T.

Since the heat transferred is the same, Equations (1-8) and (1-9) are set equal and like terms are cancelled. After some rearrangement,

$$H_v = \frac{2 ah}{b^2} . \quad (1-10)$$

The void fraction of the unit cell is defined as

$$B = \frac{\pi b^2 \Delta x - \pi a^2 \Delta x}{\pi b^2 \Delta x} = \frac{b^2 - a^2}{b^2} . \quad (1-11)$$

Rearranging Equation (1-11) and substituting in Equation (1-10), the volumetric heat transfer coefficient is defined as

$$H_V = \frac{2 (1-B)h}{a} . \quad (1-12)$$

Equation (1-9) may be rewritten in terms of a heat dissipation admittance for use later in the heat transfer network,

$$Q_V = Y_H (T - T_0) \quad (1-13)$$

where

$$\begin{aligned} Y_H &= \text{the heat dissipation admittance, } H/\theta T, \\ &= H_V S_{\text{node}} \Delta x \end{aligned} \quad (1-14)$$

$$S_{\text{node}} = \text{the cross-sectional area of a node, } L^2 .$$

Substituting from Equation (1-12), Equation (1-14) may be written as

$$Y_H = \frac{2 (1-B)h}{a} S_{\text{node}} \Delta x . \quad (1-15)$$

The heat transfer coefficient for natural convection was determined from McAdams' equation for liquids heated outside single horizontal tubes,⁽¹⁶⁾

$$\frac{hD}{k} = 0.525 \left[\left(\frac{D^3 \rho^2 \beta g (\Delta t)}{\mu^2} \right) \left(\frac{C_p \mu}{k} \right) \right]^{0.25} \quad (1-16)$$

where

- D = pin diameter, L
- k = coolant thermal conductivity, H/θLT
- ρ = coolant density, M/L³
- β = thermal coefficient of expansion of the coolant, 1/T
- g = acceleration of gravity, L/θ²
- Δt = temperature difference, T
- μ = absolute viscosity of the coolant, M/Lθ
- C_p = specific heat of the coolant, H/MT.

Stoever⁽¹⁶⁾ has evaluated Equation (1-16) for various liquids and gases, and has presented the results as a base heat transfer coefficient, which is a function of the temperature difference between the tube surface and the coolant. These results are plotted as straight lines on log-log plots and can be represented by the equation

$$h_o = B(|\Delta t|)^A \quad (1-17)$$

where

- h_o = the base heat transfer coefficient, $H/\theta L^2 T$
- A = a constant representing the slope of the straight line on a log-log plot of h_o vs Δt ,
- B = a constant representing the y-intercept of the straight line on the log-log plot of h_o vs Δt .

For liquids, the base coefficient of Equation (1-17) is multiplied by temperature and diameter correction factors to give the heat transfer coefficient for a specific film temperature and tube size,

$$h = h_o F_t F_d \quad (1-18)$$

where

- F_t = the temperature correction factor
- F_d = the diameter correction factor.

These factors are also presented in Reference 16. The temperature correction factor is a function of the film temperature as defined by

$$F_t = f(T_f) \quad (1-19)$$

and

$$T_f \approx 1/2(T_s + T_c) \quad (1-20)$$

where

$$\begin{aligned}T_f &= \text{the film temperature, } T \\T_s &= \text{the tube surface temperature, } T \\T_c &= \text{the coolant temperature, } T.\end{aligned}$$

The diameter correction factor is a function of the tube diameter as defined by

$$F_d = f(d) \quad (1-21)$$

where

$$d = \text{the tube diameter, } L.$$

Equivalent forms of Equations (1-17) through (1-21) are programmed into the model to provide the correct heat transfer coefficient during the iterative computation of the temperatures in the cask.

Unfortunately, one of the fluids not included on Stoevers' charts was Dowtherm-A. The following procedure was used to place a line on the log-log plot to represent Dowtherm-A as a first approximation. Using a correlation from Reference 2 and Dowtherm properties at 350°F, the heat transfer coefficient was obtained from

$$h = 57.4 \Delta t^{1/3}. \quad (\text{Reference 2}) \quad (1-22)$$

Assuming a value of Δt , h was determined. Using the proper diameter correction factor, and assuming that a temperature correction factor for water at 350°F would be a reasonable approximation, a value of the base coefficient was determined from Equation (1-18). This value of h_0 was then marked on the log-log plot at the Δt selected, and a line passing through this point was drawn parallel to the other lines on the plot. This line was then used for Dowtherm-A. Also, a constant average temperature correction factor of 1.0 was used throughout the study.

1.3 Heat Conduction and Apparent Thermal Conductivity

The fuel assemblies in the casks were considered to be porous bodies. The apparent thermal conductivity for a porous body may be determined from the Maxwell equation⁽¹⁶⁾

$$k_a = k_s \left[\frac{1 - (1 - \alpha \frac{k_p}{k_s})B}{1 + (\alpha - 1)B} \right] \quad (1-23)$$

where

k_a = the apparent thermal conductivity of the fuel assembly,
H/θLT,

k_s = the thermal conductivity of the solid material or fuel,
H/θLT,

k_p = the thermal conductivity of the material in the pores,
H/θLT,

$$\alpha = \frac{3 k_s}{2k_s + k_p} \cdot$$

For a coolant-filled fuel assembly, k_p would be the thermal conductivity of the coolant.

2. CASK SIMULATION MODELS FOR CALCULATION OF RATE OF COOLANT LOSS

In the opening paragraphs of this Appendix it was pointed out that the "coolant loss rate" models evolved from so-called "no-loss-of-coolant" models. The "no-loss-of-coolant" label was applied very early in the study when the primary function of the models was to determine conditions in the casks after an accident and fire, if the primary coolant was not lost. The label was applied as a logical reference to a model whose primary function was the opposite of that of the "loss-of-coolant" models.

The no-loss-of-coolant models were originally developed to determine conditions in the casks following an accident in which the casks lost their solar shields, lost the water in their outer jackets, were subjected to a 0.5-hour petroleum fire at 1475°F, but did not lose any primary coolant. It was also assumed that the pressure relief systems were inoperable. The objective was to determine the new, higher steady-state temperatures that would be reached. The new steady-state condition in the AMCO cask presented no problem since its primary coolant is Dowtherm-A, a coolant with a vapor pressure about equal to atmospheric pressure at its new higher steady-state temperature. However, the LWR cask considered (the conceptual cask in this early stage of the study) used water as a coolant, consequently its internal pressure reached an intolerably high level.

In the early stages of the study, it was assumed that the casks lost their primary coolant instantaneously at impact and were subjected to a petroleum fire at 1475°F. This led to the development of the "loss-of-coolant" models. However, it was difficult to conceive of an accident situation severe enough to cause a breach in the primary coolant containment, since these casks are extremely well-designed. Also, results from various experimental programs, including 30-foot drop tests, puncture tests, etc., in which cask models were used, indicated that the chances of a cask containment being breached in this manner would be extremely small. It seemed reasonable to assume, however, that any access to the primary coolant which had been included as part of the cask design, such as pressure relief passages and valves, fill passages and valves, etc., would have the potential for allowing coolant to escape. Since the function of

the pressure relief valve is to automatically respond to changes in the coolant-filled cask cavity, it seemed reasonable to assume that this access to the coolant would be the most likely candidate for a breach-causing failure. It was assumed that this valve could be jarred into a partially open position at impact, or it could fail to reseal after performing its function during normal operating conditions. Also, as an upper limit on postulated damage, it was assumed that the valve could be sheared off entirely. This assumption, however, does not mean that the valve's shearing off is considered at all likely. On the contrary, the pressure relief valve is a well-designed and proven component of the IF-300 cask, and is also well-protected in the IF-300 design. Breaches of this type would result in gradual rather than instantaneous loss of coolant. Consequently, the "no-loss-of-coolant" models were modified to determine the rate at which the coolant would be lost from a breach.

There are two possible mechanisms for the loss of primary coolant from a cask. These two mechanisms depend upon the final orientation of the cask after the accident. At impact, if the tiedowns fail, the cask may become separated from the rail car and come to rest in one of four positions:

1. On end with the breach up (damaged pressure relief valve),
2. On end with the breach down,
3. On its side with the breach up, and
4. On its side with the breach down.

If the tiedowns do not fail at impact, the cask will remain in its original orientation on the rail car, i.e., on its side as in positions 3 and 4 above. The first mechanism for coolant loss depends on the cask being oriented in either positions 2 or 4. In these positions, the coolant may leak out under the driving force of its own liquid head and the static pressure in the cask. The second mechanism for coolant loss depends on the cask being oriented in positions 1 and 3. In these positions the height of the coolant column would not be a driving force, but the coolant would be driven from the cask by its static pressure and by vaporization as it absorbs the decay heat from the fuel.

At impact, when a breach might be opened in a cask, the temperatures in the cask would be the steady-state temperatures determined from the pre-accident models. For the IF-300, the temperatures of the fuel, coolant inside the fuel cans, fuel cans, and coolant outside the fuel cans at this time were 361°F, 360°F, 350°F and 333°F, respectively. An average of the water temperatures is 347°F, with a corresponding vapor pressure of 130 psia. This pressure is almost 9 times atmospheric pressure, therefore this cask was treated as a pressure vessel. In the AMCO cask, the temperatures of the fuel, coolant inside the fuel cans, fuel cans, and coolant outside the fuel cans at impact were 383°F, 380°F, 364°F and 343°F, respectively. An average of the Dowtherm-A temperatures is about 360°F, with a corresponding saturation pressure of about 2.0 psia. This means that the Dowtherm is subcooled since the saturation pressure is well below atmospheric pressure. It is not likely that the pressure in the cask would be less than that of the surroundings.

2.1 Rate of Coolant Loss From the IF-300

The coolant loss rate model developed for the IF-300 is based on energy and mass balances on the cask, and on an energy balance on the breach. The main driving force causing the coolant to flow from the cask through the breach is the buildup of static pressure in the cask cavity. This pressure buildup is partly due to that portion of the decay heat from the fuel stored in the liquid and vapor phases of the coolant during the transient, and partly due to the choked flow in the breach. The breach down version of this model is developed in Section 2.1.1, and the breach up version in Section 2.1.2.

2.1.1 Coolant Loss From the Cask While in a Breach Down Position

A MIMIC listing of the breach down version of the coolant loss rate model of the IF-300 is presented in Figure 2-3.

2.1.1.1 Energy Balance on the Breach

An energy balance on the breach, in terms of a unit mass of coolant flowing, yields the First Law of Thermodynamics for a steady flow process

$$dE = J\delta Q - \delta W \quad (2-1)$$

or

$$Jde + d\left(\frac{U^2}{2g_c}\right) + \frac{g}{g_c} dZ + d(pv) = J\delta Q - \delta W \quad (2-2)$$

where

dE = the change in the total energy of the fluid, $\frac{L-F}{M}$

δQ = the increment of heat added to the fluid, $\frac{H}{M}$

δW = the increment of work done by the fluid, $\frac{L-F}{M}$

de = the change in the internal energy of the fluid, $\frac{H}{M}$

U = the velocity of the fluid, $\frac{L}{\theta}$

g_c = the gravitational constant, $\frac{ML}{F\theta^2}$

g = the local acceleration of gravity, $\frac{L}{\theta^2}$

dZ = the change in the height of the fluid, L

$d\left(\frac{U^2}{2g_c}\right)$ = the change in the kinetic energy of the fluid, $\frac{L-F}{M}$

$d(pv)$ = the change in the flow work of the fluid, $\frac{L-F}{M}$

p = the static pressure of the fluid, $\frac{F}{L^2}$

v = the specific volume of the fluid, $\frac{L^3}{M}$

J = the mechanical equivalent of heat, $\frac{L-F}{H}$.

By definition

$$Jde = Jdh - pdv \quad (2-3)$$

Using Equation (2-3), and assuming that

$$\delta W = 0,$$

Equation (2-2) may be changed to

$$Jdh - pdv + d\left(\frac{U^2}{2g_c}\right) + \frac{g}{g_c} dZ + pdv + vdp = J\delta Q - \delta W \quad (2-4)$$

or

$$Jdh + d\left(\frac{U^2}{2g_c}\right) + \frac{g}{g_c} dZ + vdp = J\delta Q. \quad (2-5)$$

An energy balance on the unit mass of fluid, using a frame of reference moving with the fluid, yields the First Law for a non-flow process,

$$Jde = J\delta Q_T - pdv \quad (2-6)$$

where

pdv = the total compression effects

$J\delta Q_T$ = the total thermal effects from all sources, including friction, etc.

The total thermal effects may be expressed as

$$J\delta Q_T = J\delta Q + J\delta F \quad (2-7)$$

where

δF = the heat added due to friction

δQ = the heat added from all other sources other than friction.

Combining Equations (2-6) and (2-7) gives

$$Jde = J\delta Q + J\delta F - pdv. \quad (2-8)$$

Substituting from Equation (2-3) and cancelling like terms, Equation (2-8) may be written as

$$Jdh = J\delta Q + J\delta F. \quad (2-9)$$

Finally, substituting from Equation (2-9) into (2-5) gives the mechanical energy balance

$$d\left(\frac{U^2}{2g_c}\right) + \frac{g}{g_c} dZ + vdp = -J\delta F. \quad (2-10)$$

The maximum rate of loss and the minimum time required to empty the cask would occur if it is assumed that the flow of fluid from the breach is isentropic, i.e.,

$$J\delta F = 0. \quad (2-11)$$

Using the condition defined by Equation (2-11), the energy balance (2-10) reduces to

$$d\left(\frac{U^2}{2g_c}\right) + \frac{g}{g_c} dZ + vdp = 0. \quad (2-12)$$

Since $g = g_c$ under normal conditions, Equation (2-12) may be rearranged to yield

$$d\left(\frac{U^2}{2g_c}\right) = -dZ - vdp \quad (2-13)$$

or, in terms of the density rather than the specific volume,

$$d\left(\frac{U^2}{2g_c}\right) = -dZ - \frac{dp}{\rho_w} \quad (2-14)$$

where $\rho_w =$ the density of the fluid, $\frac{M}{L^3}$.

Integrating from the inside of the cask to the breach exit, assuming that the density of the fluid flowing is the same as that inside the cask, gives

$$\int_{U_i}^{U_o} d\left(\frac{U^2}{2g_c}\right) = - \int_{Z_w}^0 dZ - \frac{1}{\rho_w} \int_P^{P_{ATM}} dp \quad (2-15)$$

or

$$\frac{U_o^2 - U_i^2}{2g_c} = Z_w + \frac{P - P_{ATM}}{\rho_w} \quad (2-16)$$

$$= Z_w + Z_p \quad (2-17)$$

where

$$Z_p = \frac{P - P_{ATM}}{\rho_w} \quad (2-18)$$

= the height or head of fluid of density ρ_w equivalent to the difference between the static pressure in the cask and that at the exit of the breach, L (the units of Z_p are actually $\frac{L-F}{M}$, but since $g = g_c$, the density is equivalent to a specific weight in units of $\frac{F}{L^3}$, i.e., $\gamma = \rho \frac{g}{g_c}$)

Z_w = the height of the coolant column, L

P = the static pressure inside the cask, $\frac{M}{L^3}$

P_{ATM} = the static pressure at the breach exit (atmospheric pressure), $\frac{F}{L^2}$

ρ_w = the density of the liquid coolant in the cask, $\frac{M}{L^3}$.

The height of the liquid coolant column is

$$Z_w = \frac{M_w}{\rho_w A_{CASK}} \quad (2-19)$$

where

M_w = the mass of the liquid coolant in the cask, M

A_{CASK} = the cross-sectional area of the free space in the cask, L^2 .

The cross-sectional area of the free space in the cask is determined from initial conditions and the equation

$$A_{\text{CASK}} = \frac{M_{wi}}{\rho_w Z_i} \quad (2-20)$$

where

M_{wi} = the initial mass of the coolant in the cask, M

Z_i = the initial height of the coolant column, L.

Setting

$$Z = Z_w + Z_p \quad (2-21)$$

and assuming that the fluid velocity inside the cask is

$$U_i \cong 0, \quad (2-22)$$

then Equation (2-16) may be expressed as

$$U_o = \sqrt{2g_c Z} \quad (2-23)$$

The mass velocity of the coolant leaving the cask is defined by

$$G = \rho_w U_o \quad (2-24)$$

or

$$G = \rho_w \sqrt{2g_c Z} \quad (2-25)$$

A set of charts has been developed by Moody⁽⁹⁾ to provide a convenient method for evaluating the maximum rate of loss of steam or water from a pressurized vessel that suffers a break in its containment. The maximum rate of loss of either the vapor or the liquid from the breach is governed by a thermodynamically defined critical or maximum mass flow rate based on isentropic flow of the fluid from the breach. A chart is presented in Reference 9, and as Figure 2-1, that relates the critical or maximum mass flow rate of steam and water to the stagnation enthalpy and pressure.

2.1.1.2 Rate of Coolant Loss From the Breach and Mass Balance on the Cask

When the cask is in a breach down position, saturated liquid would flow through the breach. The maximum mass velocity of this liquid would be obtained from the Moody chart as a function of the static or stagnation pressure in the cask

$$G_{MAXF} = f(P) \quad (2-26)$$

where

G_{MAXF} = the maximum mass velocity of the saturated liquid, $M/\theta L^2$.

If G is greater than G_{MAXF} , the flow of liquid (two-phase) through the breach is choked and the maximum rate at which fluid can flow from the breach is G_{MAXF} . Therefore, it is convenient to define a mass velocity G_{OUT} , based on both G and G_{MAXF} .

$$G_{OUT} = G \quad \text{when } G \leq G_{MAXF} \quad (2-27)$$

$$G_{OUT} = G_{MAXF} \quad \text{when } G > G_{MAXF} \quad (2-28)$$

FIGURE 2-1. Maximum Steam/Water Flow Rate and Local Stagnation Properties (Reference 9)

One of the functions available in the MIMIC simulation program is one which chooses the smallest of six values. This function, as applied to the situation defined by Equations (2-27) and (2-28), would be written as

$$G_{OUT} = \text{MIN} (G, G_{MAXF}) \quad (2-29)$$

where

G_{OUT} = the actual mass velocity of the fluid flowing from the breach, $M/\theta L^2$.

The rate of change of the mass of coolant in the cask is

$$\frac{dM_x}{dt} = - G_{OUT} A_{GAP} \quad (2-30)$$

where

A_{GAP} = the flow area of the breach, L^2 .

As coolant flows from the breach, a space filled with coolant vapor in equilibrium with the liquid is created above the liquid. The total mass of coolant remaining in the cask as a mixture of liquid and vapor is

$$M_x = - \int_0^t G_{OUT} A_{GAP} dt + M_{wi} \quad (2-31)$$

where

M_x = the total mass of coolant remaining in the cask as a mixture of liquid and vapor, M

M_{wi} = the initial mass of coolant in the cask, M.

A mass balance on the cask may be written as

$$M_{wo} = M_{wi} - M_x \quad (2-32)$$

where

M_{WC} = the mass of coolant lost, M.

The volumes occupied by the liquid and vapor portions of the coolant remaining in the cask are unknown. However, since the sum of the volumes must be equal to the total free cask volume, V_{CASK} , the average density of the liquid-vapor mixture may be defined by

$$\rho_x = \frac{M_x}{V_{CASK}} \quad (2-33)$$

where

$$V_{CASK} = Z_i A_{CASK} \cdot \quad (2-34)$$

Assuming that the mixture consists of saturated vapor and saturated liquid, the densities of each may be obtained as functions of the saturation temperature of the mixture,

$$\rho_W = f(T_W) \quad (2-35)$$

$$\rho_G = f(T_W) \quad (2-36)$$

where

ρ_G = the density of the vapor, M/L³

T_W = the saturation temperature of the mixture, T.

Using the concept of quality of a mixture of vapor and liquid, the specific volume of the mixture may be written as

$$v_x = xv_G + (1-x)v_W \quad (2-37)$$

or

$$\frac{1}{\rho_x} = \frac{x}{\rho_G} + \frac{(1-x)}{\rho_W} \quad (2-38)$$

Solving Equation (2-38) for the quality gives

$$x = \frac{\left(\frac{1}{\rho_X}\right) - \left(\frac{1}{\rho_W}\right)}{\left(\frac{1}{\rho_G}\right) - \left(\frac{1}{\rho_W}\right)} \quad (2-39)$$

where

$$x = \text{the quality of the mixture, } \frac{M_{(\text{VAPOR})}}{M_{(\text{MIXTURE})}} .$$

The masses of the liquid and vapor portions of the mixture may be obtained using the total mass of the mixture and the quality in the following equations,

$$M_V = x M_X \quad (2-40)$$

$$\text{and} \quad M_W = (1-x) M_X , \quad (2-41)$$

where

$$M_V = \text{the mass of the vapor in the mixture, } M.$$

When all of the liquid coolant is expelled from the cask, a substantial amount of vapor remains. At this point,

$$x = 1$$

$$\text{and} \quad M_V = M_X .$$

As shown in Section 2.1.1.1, Equation (2-16), the forces driving the coolant from the cask are the potential energy of the liquid column and the pressure in the cask. The pressure in the cask during most of the transient is due to the vapor portion of the mixture and is defined by the ideal gas law

$$P = \frac{M_V R (T_W + 460)}{V \text{ MOL}_V} \quad (2-42)$$

where

$$\begin{aligned} R &= \text{the gas constant, } \text{L-F}/(\text{MOLE})(\text{T}) \\ V &= \text{the volume of the vapor, } \text{L}^3 \\ \text{MOL}_V &= \text{the molecular weight of the vapor, } \text{M}/\text{MOLE}. \end{aligned}$$

Initially, if the coolant expands at a faster rate than it is lost from the cask, a vapor portion is not formed immediately. In this short initial period, the pressure is obtained from the Steam Tables⁽²⁷⁾ and expressed as the relation

$$P = f(T_W) . \quad (2-43)$$

All integrations in the MIMIC simulation program are performed by a centralized integration routine. The particular algorithm employed is a fourth order variable step Runge-Kutta method. Because of this step-wise procedure, the values of some variables may slightly "overshoot" their actual physical limits when these limits are reached during the course of the simulation. If this is not prevented, the realism of the simulation might be jeopardized. This is true of the coolant mixture quality, x , and the height Z_w of the column of liquid. The quality must be within the limits 0 and 1, and the height can only vary from Z_i to 0. During the course of the present simulation, these variables slightly overshoot these limits and produced erroneous results. This was remedied by using a MIMIC "limiter" function (see Figure 2-2). Using this limiter function, the quality may be represented by

$$X = \text{LIM} (\text{QUALITY}, 0., 1.) \quad (2-44)$$

where

$$\text{QUALITY} = \frac{\left(\frac{1}{\rho_X}\right) - \left(\frac{1}{\rho_W}\right)}{\left(\frac{1}{\rho_G}\right) - \left(\frac{1}{\rho_W}\right)} . \quad (2-45)$$

This application of the limiter function assures that

$$\begin{aligned} X &= 0, \text{ when } \text{QUALITY} < 0 \\ X &= \text{QUALITY}, \text{ when } 0 \leq \text{QUALITY} \leq 1 \\ X &= 1, \text{ when } \text{QUALITY} > 1. \end{aligned}$$

Similarly, the height of the liquid column may be represented by

$$Z_{WA} = \text{LIM}(Z_{WB}, 0., 14.) \quad (2-46)$$

where $Z_{WA} = Z_{WA}$ = an interim value of the height Z_W ,

and $Z_{WB} = Z_{WB} = \frac{M_W}{\rho_W A_{\text{CASK}}} . \quad (2-47)$

This application of the limiter assures that

$$\begin{aligned} Z_{WA} &= 0. & \text{when } Z_{WB} < 0. \\ Z_{WA} &= Z_{WB} = \frac{M_W}{\rho_W A_{\text{CASK}}} & \text{when } 0. \leq Z_{WB} \leq 14. \\ Z_{WA} &= 14. & \text{when } Z_{WB} > 14. \end{aligned}$$

The height Z_W is actually the interim value Z_{WA} and could be obtained from Equation (2-46). However, a MIMIC "implicit function" must be used to avoid a closed algebraic loop. This algebraic loop is formed because, as will be shown later, Z_W is used to determine the quality x , which is then used to determine M_W , which in turn is used to determine Z_W from Equation (2-47). The implicit function evaluates Equation (2-46) using an iterative process. The action of the implicit function is to prevent the independent variable, time, from being incremented until the difference between the last

calculated value of Z_W and the previously calculated value is less than or equal to 5×10^{-6} times the previously calculated value. The MIMIC implicit function statement for Z_W is

$$ZW = \text{IMP}(ZW, ZWA). \quad (2-48)$$

An initial value of Z_W is given on a data card corresponding to the parameter (PAR) card naming Z_W (see the model listing of Figure 2-3). See Reference 3 for a detailed discussion of the implicit function.

The nature of the coolant loss rate models dictates that the flow of computations within the models must proceed along one of several alternate paths, with the choice of path depending upon the values attained by certain key variables. The MIMIC simulation program accommodates this branching process through the use of logical control variables generated by the combination of a function switch, or one or more logical functions, and the constants TRUE and FALSE. One of the uses of a logical variable is to provide control over the execution of individual MIMIC statements or operations. If a statement or operation is flagged by a logical variable name, then the statement will be evaluated when the control variable has a "true" value and not when the control variable has a "false" value. This means that the logical control variable can be used to select, under program control, which of several statements should be evaluated. This use of a logical control variable generated by a function switch or logical function serves the same function as the conditional transfer statements in FORTRAN, i.e., the IF and computed GO TO statements. Specific uses of logical control variables to achieve branching within the coolant loss rate models will be presented in the remainder of this sub-section for the breach down version, and in Section 2.1.2 for the breach up version. See Reference 3 for a detailed explanation of the use of logical control variables in MIMIC programming. A summary of the functions available in MIMIC, including the logical control variables, is presented in Figure 2-2.

It was assumed that, at the time a breach is opened in the cask containment, the cavity contains only liquid coolant, i.e., no vapor space

C	SUBROUTINE MIMCO	MIMIC
C	COMPILER	MIMIC
C	DEFINITIONS	MIMIC
C	DEFINITION OF TERMS	MIMIC
C	GE=GREATER THAN OR EQUAL TO	MIMIC
C	LE=LESS THAN OR EQUAL TO	MIMIC
C	GT=GREATER THAN	MIMIC
C	EQ=EQUAL TO	MIMIC
C	LOGICAL CONTROL VARIABLE (LCV)	MIMIC
C	IF A LOGICAL CONTROL VARIABLE IS ENTERED IN COLUMNS 2-7, THAT	MIMIC
C	OPERATION WILL BE EXECUTED IF THE VARIABLE IN COLUMNS	MIMIC
C	2-7 IS TRUE AND SKIPPED IF IT IS FALSE.	MIMIC
C	LITERALS	MIMIC
C	FIXED POINT LITERALS ARE PERMITTED IN MIMIC. THEY MAY CONTAIN	MIMIC
C	NO MORE THAN SIX SYMBOLS, ONE OF WHICH MUST BE A DECIMAL POINT.	MIMIC
C	NAMES	MIMIC
C	ALL NAMES IN MIMIC CONSIST OF FROM ONE TO SIX	MIMIC
C	ALPHANUMERIC CHARACTERS.	MIMIC
C	SPECIAL NAMES	MIMIC
C	T THE INDEPENDENT VARIABLE	MIMIC
C	DT PRINT INTERVAL	MIMIC
C	DTMAX MAXIMUM INTEGRATION STEP SIZE	MIMIC
C	DTMIN MINIMUM INTEGRATION STEP SIZE	MIMIC
C	TRUE	MIMIC
C	FALSE	MIMIC
C	FORMAT OF OPERATIONS	MIMIC
C	COLUMN 1 ANY SYMBOL IN COLUMN 1 DENOTES A COMMENT CARD.	MIMIC
C	COLUMNS 2-7 LOGICAL CONTROL VARIABLE	MIMIC
C	COLUMNS 10-15 RESULT	MIMIC
C	COLUMNS 19-72 EXPRESSION	MIMIC
C	COLUMNS 73-80 COMMENTS OR IDENTIFICATION	MIMIC
C	DATA FORMAT	MIMIC
C	CONSTANTS 6E12.0	MIMIC
C	PARAMETERS 6E12.0	MIMIC
C	FUNCTIONS 2E12.0/3E12.0	MIMIC
C	ALL CONSTANTS MUST COME BEFORE THE FIRST PARAMETER.	MIMIC
C	*** OPTIONS ***	MIMIC
C	COL.1234567890123456789.....	MIMIC
C	ELIST LISTS VALUES FOR VARIABLES AT END OF RUN	MIMIC
C	DELETE SKIPS MACHINE FUNCTION SET-UP LISTING	MIMIC
C	ABSEERR XXXXXX USES ABS. ERROR OF XXXXXX FOR INTEGRATION	MIMIC
C	LIST OF MIMIC FUNCTIONS	MIMIC

FIGURE 2-2. Summary of Rules and Functions of MIMIC, A Continuous System Simulation Program (Page 1 of 4)

FUNCTION	CODE INPUT(S)	OUTPUT/REMARKS	MIMIC
ABSOLUTE VALUE	ABS A	R=ABS(A)	MIMIC
ARCCOSINE	ACS A	R=ARCCOS(A)	MIMIC
ADDITION	ADD A,B (,C,D,E,F) SUM	R=A+B (+C(+D(+E(+F))))	MIMIC
AND	AND A,B (,C,D,E,F)	R=TRUE IF A AND B(ETC.)TRUE. R=FALSE OTHERWISE	MIMIC
ARCSINE	ASN A	R=ARCSIN(A)	MIMIC
ARCTANGENT	ATN A,B	R=ARCTAN(A/B). B IS ASSUMED +1. IF NOT SPECIFIED.	MIMIC
NAME FUNCTION (CONSTANT)	CEN A	R=NAME OF ARRAY. A=NO. OF PAIRS OF POINTS.	MIMIC
LOGICAL COMPLEMENT	COM A NOT	R=TRUE IF A FALSE. R=FALSE IF A TRUE.	MIMIC
NAME CONSTANTS	CCN A,B,C,D,E,F	ENTERS CONSTANT NAMES	MIMIC
COSINE	COS A(RADS)	R=COS(A)	MIMIC
HYPERBOLIC COSINE	CSH A	R=COSH(A)	MIMIC
DERIVATIVE	DER A,B,C	R=DB/DA R=C AT T=0.	MIMIC
DIVIDE	DIV A,B	R=A/B	MIMIC
DEAD SPACE	DSP A,B,C	R=A-B IF A LT B R=0 IF B LE A LE C R=A-C IF A GT C	MIMIC
END OF PROGRAM	END		MIMIC
EXCLUSIVE OR	EOR A,B	R=TRUE IF A TRUE AND B FALSE OR IF A FALSE AND B TRUE. R=FALSE OTHERWISE	MIMIC
EQUALITY	EQL A	R=A	MIMIC
EXPONENTIATION	EXP A (,B)	R=B**A. E=2.781.. IS ASSUMED FOR UNSPECIFIED B.	MIMIC
GO TO NEXT CASE	FIN A,B	GO TO NEXT CASE IF A GE B	MIMIC
TRUNCATION	FIX A	R=INTEGER PART OF A.	MIMIC
FLIP-FLOP	FLF A,B,C	R=TRUE IF (A TRUE) OR (B FALSE AND R TRUE). R=FALSE OTHERWISE. AT T=0. R=C.	MIMIC

FIGURE 2-2. Summary of Rules and Functions of MIMIC, A Continuous System Simulation Program (Page 2 of 4)

C	FUNCTION SWITCH	FSW A,B,C,D	R=B IF A LT 0. R=C IF A EQ 0. R=D IF A GT 0.	MIMIC
C				MIMIC
C				MIMIC
C				MIMIC
C	FIRST ORDER	FTR A,B	R=INVERSE LAPLACE TRANSFORM	MIMIC
C	TRANSFER FUNCTION		(1/(BS+1))A(S)	MIMIC
C				MIMIC
C	FUNCTION	FUN A,B	R=A(B)	MIMIC
C	FUNCTION	FUN A,B,C	R=A(B,C)	MIMIC
C				MIMIC
C	HEADER	HDR A,B,C,D,E,F	PRINT HEADING NAMES	MIMIC
C		HEA		MIMIC
C				MIMIC
C	IMPLICIT FUNCTION	IMP A,B(A)	R=A WHERE A-B(A)=0	MIMIC
C				MIMIC
C	INTEGRATION	INT A,B(C,D)	R=B+INT(A) C FALSE D FALSE OPERATE C FALSE D TRUE HOLD C TRUE D FALSE RESET C TRUE D TRUE OPERATE	MIMIC
C				MIMIC
C	INCLUSIVE OR	IOR A,B(C,D,E,F)	R=TRUE IF A OR B(ETC.)TRUE. R=FALSE OTHERWISE	MIMIC
C				MIMIC
C	LIMITER	LIM A,B,C	R=0 IF A LT B R=A IF B LE A LE C R=C IF A GT C	MIMIC
C				MIMIC
C	LIMIT INTEGRATORS	LIN A,B,C,D	R=DERIVATIVE OF B, WHERE B IS THE LIMITED INTEGRATOR OUTPUT(C LE B LE D).A IS THE DERIVATIVE OF UNLIMITED B.	MIMIC
C				MIMIC
C	LOGARITHM	LOG A(B)	R=LOG(A),BASE B (ASSUMED AS ABOVE IF NOT SPECIFIED)	MIMIC
C				MIMIC
C	LOGICAL SWITCH	LSW A,B,C	R=B IF A TRUE. R=C IF A FALSE.	MIMIC
C				MIMIC
C	MULTIPLY AND ADD	MAD A,B,C(D,E,F)	R=A*B+C (*D(+E(*F)))	MIMIC
C				MIMIC
C	MAXIMUM	MAX A,B(C,D,E,F)	R=MAX(A,B(C,D,E,F))	MIMIC
C				MIMIC
C	MINIMUM	MIN A,B(C,D,E,F)	R=MIN(A,B(C,D,E,F))	MIMIC
C				MIMIC
C	MODULO	MOD A,B	R=A MODULO B = A-(A/B)*B	MIMIC
C				MIMIC
C	MONOSTABLE MULTIVIBRATOR	MMV A,B	R SET TRUE WHEN A TRUE AND STAYS TRUE FOR B SECONDS AFTER A GOES FALSE. R=A AT T=0.	MIMIC
C				MIMIC
C	MULTIPLICATION	MPY A,B(C,D,E,F)	R=A*B (*C(*D(*E(*F)))	MIMIC
C				MIMIC
C	NEGATION	NEG A	R=-A	MIMIC
C				MIMIC
C	PRINT OUTPUT	OUT A,B,C,D,E,F PRI	PRINT A,B,C,D,E,F EVERY DT UNITS OF T.	MIMIC
C				MIMIC

FIGURE 2-2. Summary of Rules and Functions of MIMIC, A Continuous System Simulation Program (Page 3 of 4)

exists, and

$$Z_w = Z_i, \quad (2-49)$$

where Z_i = the initial height of the liquid column.

This condition also prevails initially in the transient if the coolant expands at a sufficient rate to keep the cask full of liquid, even though some of the coolant is lost from the cask. When enough coolant is lost, a vapor space is formed above the liquid and

$$0 \leq Z_w < Z_i. \quad (2-50)$$

When both liquid and vapor are present, the quality of the mixture is in the range

$$0 < x < 1. \quad (2-51)$$

When only liquid is present,

$$x = 0, \quad (2-52)$$

and, when only vapor is present,

$$x = 1. \quad (2-53)$$

Since Equations (2-51), (2-52) and (2-53) define three conditions which cannot exist at the same time, the quality must be determined from different expressions.

The local control variables that select the proper computational flow paths for the conditions defined by Equations (2-49) and (2-50) are XOFF and XON, respectively. XOFF is defined by the function switch expression

$$XOFF = FSW(ZW-ZI, FALSE, TRUE, TRUE) \quad (2-54)$$

where $ZW = Z_w$

$$ZI = Z_i,$$

and XON is defined by the logical complement of XOFF

$$XON = \text{NOT}(XOFF). \quad (2-55)$$

When Equation (2-49) is true, XOFF is true and XON is false. If XOFF is true, any expression flagged by this logical control variable is evaluated. There are two equations in the model that define the quality x . One of these is Equation (2-52), which is flagged by XOFF to give

$$XOFF \quad X = 0. \quad (2-56)$$

where $X = x$.

The second expression is Equation (2-44), which is flagged by XON to give

$$XON \quad X = \text{LIM}(\text{QUALTY}, 0., 1.) \quad (2-57)$$

where QUALTY is defined by Equation (2-45). When Equation (2-50) is true, XOFF is false and XON is true, and Equation (2-57) is evaluated instead of Equation (2-56).

The pressure in the cask is also determined by two different equations, depending upon whether or not vapor is present. If vapor is present, the pressure is defined by Equation (2-42). If the cask contains only liquid, the pressure is defined by Equation (2-43). To select the appropriate equation, it was convenient to establish the function switch expression

$$XPAND = \text{FSW}(X, \text{TRUE}, \text{TRUE}, \text{FALSE}) \quad (2-58)$$

and its logical complement

$$\text{CNTRCT} = \text{NOT}(XPAND). \quad (2-59)$$

When the cask is filled with liquid, Equation (2-56) applies and XPAND is true and CNTRCT is false. Therefore, Equation (2-43) is flagged by XPAND to give

$$\text{XPAND} \quad P = \text{FUN}(\text{PSAT}, \text{TW}) \quad (2-60)$$

where the equation is written as a MIMIC function expression (see Figure 2-2 and Reference 3). If the cask is filled with a mixture of liquid and vapor, or with vapor only, Equation (2-57) applies to make XPAND false and CNTRCT true. In this case, Equation (2-42) is flagged by CNTRCT to give

$$\text{CNTRCT} \quad P = \text{MV} * \text{R} * (\text{TW} + 460.) / (\text{MOLV} * \text{V} * 144.) \quad (2-61)$$

where the equation is expressed in FORTRAN notation as programmed for MIMIC.

While liquid coolant is in the cask, the vapor volume is defined by

$$V = \frac{M_v}{\rho_G} \quad , \quad (2-62)$$

but when all of the liquid is expelled from the cask, the vapor volume is defined by

$$V = V_{\text{CASK}} \quad . \quad (2-63)$$

The following equations are valid only while liquid coolant is in the cask:

$$Z_p = \frac{P - P_{\text{ATM}}}{\rho_w} \quad (2-18)$$

$$G = \rho_w \sqrt{2g_c Z} \quad (2-25)$$

$$G_{\text{OUT}} = \text{MIN}(G, G_{\text{MAXF}}) \quad (2-29)$$

and

$$V = \frac{M_v}{\rho_G} \quad . \quad (2-62)$$

Corresponding equations, which are valid only when all of the liquid coolant has been expelled from the cask, are written for the vapor in the cask and for vapor flowing through the breach:

$$Z_p = \frac{(P - P_{ATM})}{\rho_G} \quad (2-64)$$

$$G = \rho_G \sqrt{2g_c Z} \quad (2-65)$$

$$G_{OUT} = \text{MIN}(G, G_{MAXG}) \quad (2-66)$$

and $V = V_{CASK} , \quad (2-63)$

where

$$G_{MAXG} = f(P) \quad (2-67)$$

is the maximum mass velocity of the saturated vapor flowing through the breach. Since these two sets of equations cannot be used at the same time, the computation flow must be divided into two branching paths at this point.

As discussed earlier, control of computation flow in a model programmed in the MIMIC simulation language is accomplished by the use of logical control variables. The model presented here was constructed to determine conditions in and the rate of coolant loss from the cask both before and after the liquid coolant has been expelled, i.e.,

$$M_w > 0 \quad (2-68)$$

and

$$M_w \leq 0, \quad (2-69)$$

respectively. The logical control variables representing the conditions defined by Equations (2-68) and (2-69) are CLNT and EMPTY, respectively. CLNT is defined by the function switch expression

$$CLNT = FSW(MW, FALSE, FALSE, TRUE) \quad (2-70)$$

and EMPTY by the logical complement of CLNT

$$EMPTY = NOT(CLNT). \quad (2-71)$$

When Equation (2-68) is true, CLNT is true and EMPTY is false. Conversely, when Equation (2-69) is true, CLNT is false and EMPTY is true. These control variables are to be used only when the cask contains either a mixture of liquid and vapor, or vapor only. Therefore, they must, in turn, be flagged by the logical control variable CNTRCT defined by Equation (2-59):

$$CNTRCT \quad CLNT = FSW(MW, FALSE, FALSE, TRUE) \quad (2-72)$$

$$CNTRCT \quad EMPTY = NOT(CLNT) \quad (2-73)$$

The use of all the logical control variables presented in this section is illustrated in the MIMIC listing of the model in Figure 2-3.


```

*
IFCLR
*
*   BREACH UP *****
*
      CON(MWI,PI,VI,AGAP,TWI,XI)
      CON(ZI,GC,PATM)
      CON(Q,MOLV,R)
      CON(J)
      CON(KHV,U,DJ,KHJS,DB)
      CON(CC1,CC2,CB,K,F,CPG)
      CON(TCI,TJ1,TB1)
      CON(KHFV,TF1,CF)
      RHO = CFN(4.)
      GMAX = CFN(6.)
      GMAXV = CFN(6.)
      HFG = CFN(6.)
      FPF = CFN(7.)
      TSF = CFN(4.)
      HR = CFN(16.)
      FPFVF = CFN(7.)
      HWF = CFN(6.)
      HGF = CFN(6.)
      RHOG = CFN(6.)
      PSAT = CFN(11.)
      PAR(TJC)
      PAR(ZW)
      TEO = FSW(T,TRUE,TRUE,FALSE)
      TGTU = NOT(TEO)
      TEO ACASK = MWI/(RHO*ZI)
      RHO = FUN(RHO,TW)
      HVAP = FUN(HFG,F)
      TEO VCASK = ACASK*ZI
      CLNT = FSW(MW,FALSE,FALSE,TRUE)
      EMPTY = NOT(CLNT)
      XPAND P = FUN(PSAT,TW)
      CNTRCT P = MV*K*(TW+460.)/(MOLV*V*144.)
      CLNT V = MV/RHOG
      EMPTY V = VCASK
      DTF = (Q-YV*(TF-TW))/CF
      DTW = (YV*(TF-TW)-Y1*(TW-TC))/CMIX
      DTC = (Y1*(TW-TC)-Y2*(TC-TJ))/CC1
      DTJ = (Y2*(TC-TJ)-Y3*(TJ-TB)-Y5*(TJ-TJC))/CC2
      DTB = (Y3*(TJ-TB)-Y4*(TB-TS)+Y6*(TJ-TB))/CB
      TF = INT(DTF,TF1)
      TW = INT(DTW,TW1)
      TC = INT(DTC,TC1)
      TJ = INT(DTJ,TJ1)
      TB = INT(DTB,TB1)
      TS = FUN(TSF,T)
      TJC = IMP(TJC,(Y5*TJ+Y6*TB)/(Y5+Y6))
      CMIX = CPG*RHOG*V+MW
      YV = YVG+YVW
      YVW = 173.*ZW*HFL
      YVG = 173.*(ZI-ZW)*HFV
      HFL = .0133*EXP(.25,ABS(TF-TW))
      HFV = KHFV*FPFV*EXP(.256,ABS(TF-TW))
      FPFV = FUN(FPFVF,P)
      RHOG = FUN(RHOG,TW)

```

FIGURE 2-3. MIMIC Listing of the Coolant Loss Rate Model of the IF-300 (Breach Down Version) (Page 1 of 3)

```

Y1      = 3.14*D*((ZI-ZW)*HV+ZW*HL)
HL      = .0089*EXP(.3355,ABS(TW -TC))
HV      = KHV*FP*EXP(.375,ABS(TW -TC))
FP      = FUN(FPF,P)
Y2      = 3.14*(D+DJ)*ZI*K/(DJ-D)
Y3      = 3.14*F*DJ*ZI*HRJB
HRJB    = FUN(HR,TJ,TB)
Y5      = 3.14*DJ*ZI*HJS
HJS     = KHJS*EXP(.375,ABS(TJ-TJC))
Y6      = 3.14*DB*ZI*HSB
HSB     = KHJS*EXP(.375,ABS(TJC-TB))
Y4      = 3.14*DB*ZI*(HBO+HRO)
HBO     = KHJS*EXP(.375,ABS(TB-TS))
HRO     = FUN(HR,TB,TS)
GMAXF   = FUN(GMAX,P)
GMAXG   = FUN(GMAXV,P)
CLNT    GOUT  = MIN(G,GMAXF)
EMPTY   GOUT  = MIN(G,GMAXG)
RHOX    = MX/VCASK
XOFF     = FSW(ZW-14.,FALSE,TRUE,TRUE)
XUN      = NOT(XOFF)
XOFF     X      = 0.
DMX      = -GOUT*AGAP/144.
MX       = INT(DMX,MWI)
MWO      = MWI-MX
QUALITY  = (1./RHOX-1./RHOW)/(1./RHOG-1./RHOW)
XUN      X      = LIM(QUALITY,0.,1.)
XPAND    = FSW(X,TRUE,TRUE,FALSE)
CNTRCT   = NOT(XPAND)
MV        = X*MX
MW        = (1.-X)*MX
CLNT     G      = RHOW*SQR(2.*GC*Z)
EMPTY    G      = RHOG*SQR(2.*GC*Z)
QRAD     = Y1*(TW-TC)
QOUT     = QRAD
QIN      = YV*(TF-TW)
QNET     = QIN-QOUT
Z         = ZW+ZP
ZWA      = LIM(MW/(RHOW*ACASK),0.,14.)
ZW       = IMP(ZW,ZWA)
CLNT     ZP     = (P-PATM)*144./RHOW
EMPTY    ZP     = (P-PATM)*144./RHOG
DT        = 10.
HOURS    = T/3600.
FIN(PATM,P)
FIN(T,43200.)
OUT(T,MW,MWO,GMAXF,G,GOUT)
OUT(HOURS,ZP,ZW,Z,MV,X)
OUT(,MX,HVAP,MVT,GMAXG)
OUT(,P,V,VO)
OUT(,Z,QUALITY)
OUT(,RHOW,RHOG,RHOX)
TEO      OUT(,MWI,VCASK,ACASK)
OUT(,QGAP,QRAD,QIN)
OUT(,QOUT,QNET)
OUT(,TF,TW,CMIX,CPG)
OUT(,TC,TJ,TB,TS,TJC)
OUT(,YV,YVW,YVG)
OUT(,Y1,Y2,Y3,Y5,Y6)
OUT(,Y4,HL,HV,FP,HJS)
OUT(,HFL,HFW,FPFV,HW,HG)
OUT(,HSB,HBO,HRJB,HRO)
OUT

```

FIGURE 2-3. MIMIC Listing of the Coolant Loss Rate Model of the IF-300 (Breach Down Version) (Page 2 of 3)

```

OUT
OUT
PLU(T,TF,TW,TC,TJ,  TB)
PLU(T,TJC,TS)
PLU(T,MW,MWO,ZW,P,X)
PLU(T,MX)
PLU(T,GMAXF,G,GOUT,GMAXG)
END

```

FIGURE 2-3. MIMIC Listing of the Coolant Loss Rate Model of the IF-300
(Breach Down Version) (Page 3 of 3)

2.1.1.3 Energy Balances on the Cask and the Determination of Temperatures

The densities of the liquid and vapor phases of the coolant in the cask, and the pressure in the cask, are functions of the coolant temperature. The maximum mass velocities of the liquid and vapor flowing from the breach are, in turn, functions of the pressure. The coolant temperature was obtained as a function of time, along with some other temperatures in the cask, from a set of energy balances on various regions of the cask.

An idealized representation of the cask, shown as an electrical analog in Figure 2-4, was used to construct a heat transfer sub-model. This idealized model of the IF-300 consists of four regions represented by seven nodes, for which energy balances were written to form the sub-model. The four regions are:

1. The fuel assemblies as one homogeneous region, represented by one node,
2. The coolant in the cask cavity, represented by one node,
3. The cask wall (steel and uranium), represented by two nodes, one at the inner surface and one at the outer surface, and
4. The outer water jacket, represented by two nodes, one for the vapor in the jacket and one representing the outer corrugated shell.

The seventh node represents the temperature of the surroundings (including the 0.5-hour fire).

Heat enters the cask as decay heat generated in the fuel and as heat input from the fire. Heat leaves the cask by natural convection and radiation from the cask surface to the surroundings, and in the coolant lost from the cask. Solar heat input was neglected since the time required to empty the cask was expected to be small enough that the effects of solar heating would be negligible.

Initial temperatures in the cask are obtained from the temperature distribution established by the steady-state pre-accident model.

HEDL 7507-30.5

FIGURE 2-4. Idealized Representation of the IF-300 as an Electrical Analog

The temperature of the surroundings is a function of time. During the fire, it is the temperature of the fire and, when the fire burns out, it becomes the ambient temperature of the surroundings. This variation of the temperature is programmed into the model as a time-varying step function.

It is convenient to define and discuss in general, beforehand, some of the terms to be used in the energy balance equations.

2.1.1.3.1 Thermal Admittances, Heat Transfer Coefficients, Thermal Capacities and Heat Generation

Since the purpose of the coolant loss rate model was to provide estimates of the time required for the cask to lose its coolant, no attempt was made to determine detailed temperature distributions in the cask. Consequently, all but one of the thermal admittances in the heat balance equations are for heat transfer by convection, radiation, or combined convection and radiation. The only heat conduction admittance is for the cask wall.

All convection admittances, except the one representing heat transfer from the fuel to the coolant, are defined by the general equation

$$Y_h = hA \quad (2-74)$$

where

Y_h = the admittance for heat transfer by convection, $H/\theta T$,

h = the coefficient for heat transfer by natural convection,
 $H/\theta L^2 T$,

A = the surface area for heat transfer, L^2 .

Heat transfer by natural convection from the fuel to the coolant is represented by a volumetric heat dissipation admittance which has been defined by Equation (1-15) in Section 1.2, i.e.

$$Y_v = \frac{2(1-B)h S_{node} \Delta x}{a} \quad (2-75)$$

where

- Y_v = the volumetric heat dissipation admittance, $H/\theta T$,
- B = the void fraction of the fuel region,
- h = the coefficient for heat transfer by natural convection from a fuel pin to the coolant, $H/\theta L^2 T$,
- a = the fuel pin radius, L ,
- S_{node} = the cross-sectional area of the fuel node (in this case, S_{node} is the area of the entire fuel region), L^2 ,
- Δx = the incremental length of the fuel region (in this case, Δx represents the lengths of the respective vapor-and-liquid-cooled portions of the fuel), L .

Heat conduction through the cask wall, from the cask cavity to the inside surface of the outer water jacket, was represented by the admittance

$$Y_2 = \frac{k A_{\text{WALL}}}{\Delta r} \quad (2-76)$$

where

- Y_2 = the admittance for heat transfer by conduction, $H/\theta T$,
- k = the thermal conductivity of the cask wall, $H/\theta L T$,
- Δr = the thickness of the cask wall, L
- A_{WALL} = the mean area of the cask wall, L^2 .

The thickness of the cask wall is

$$\Delta r = 1/2 (D_J - D) \quad (2-77)$$

where

- D_J = the diameter of the wall at the outer surface, L ,
- D = the diameter of the cask cavity, L .

The mean area of the cask wall is defined by

$$A_{\text{WALL}} = \frac{\pi}{2} (D + D_J) Z_i \quad (2-78)$$

where

Z_i = the length of the cask wall, L .

Admittances representing heat transfer by radiation are defined by the general equation

$$Y_r = h_r A F \quad (2-79)$$

where

Y_r = the admittance for heat transfer by radiation, $H/\theta T$,

h_r = the coefficient for heat transfer by radiation, $H/\theta L^2 T$,

A = the area of one of the surfaces, L^2 ,

F = a combined emissivity and shape factor based on the surface corresponding to A .

The coefficient for heat transfer by natural convection from a fuel pin to the coolant was obtained from McAdam's equation⁽¹⁶⁾ for liquids and gases heated outside single horizontal tubes [see Equation (1-16) of Section 1.2]. As discussed earlier in Section 1.2, Stoevers⁽¹⁶⁾ has evaluated this equation for several liquids and gases and has presented the results as a base heat transfer coefficient, h_0 , which is a function of the temperature difference between the tube surface and the coolant [see Equation (1-17)].

The base coefficient for the liquid is multiplied by temperature and diameter correction factors to obtain the heat transfer coefficient for a specific film temperature and tube size [see Equation (1-18) of Section 1.2]. For gases, an additional pressure correction factor is required. In general, the heat transfer coefficient for the gas is obtained from the equation

$$h = h_o F_t F_d F_p \quad (2-80)$$

where

- F_t = the temperature correction factor
- F_d = the diameter correction factor
- F_p = the pressure correction factor.

The factors F_t and F_d are defined by Equations (1-19), (1-20) and (1-21) in Section 1.2. The pressure correction factor F_p is a function of the pressure, P , in the cask,

$$F_p = f(P). \quad (2-81)$$

These factors are tabulated in Reference 16. Only the pressure correction factor was used in the present stage of model development. The other two factors will be used in later stages. The product of the temperature and diameter correction factors would be greater than 1.0, so not using these factors is conservative since higher fuel temperatures are obtained.

The constants A and B in Equation (1-17) were determined from the log-log plots of h_o vs Δt for water and steam in Reference 16 to give the following equations:

$$h_{FL} = 0.0133 (|T_F - T_W|)^{0.25} \quad (2-82)$$

and
$$h_{FV} = 2.22 \times 10^{-4} F_{PFV} (|T_F - T_W|)^{0.256} \quad (2-83)$$

where

$$\begin{aligned}
 h_{FL} &= \text{the coefficient for heat transfer by natural convection} \\
 &\quad \text{from the fuel to the water in the cask, B/sec-ft}^2\text{-}^\circ\text{F}, \\
 h_{FV} &= \text{the coefficient for heat transfer by natural convection} \\
 &\quad \text{from the fuel to the steam in the cask, B/sec-ft}^2\text{-}^\circ\text{F}, \\
 T_F &= \text{the fuel temperature, }^\circ\text{F} \\
 T_W &= \text{the temperature of the steam-water mixture, }^\circ\text{F}, \\
 F_{PFV} &= \text{the pressure correction factor applied to the base heat} \\
 &\quad \text{transfer coefficient for steam.} \\
 &= f(P).
 \end{aligned}
 \tag{2-84}$$

The volumetric heat dissipation admittance consists of a steam portion and a water portion

$$Y_V = Y_{VW} + Y_{VG} \tag{2-85}$$

where

$$\begin{aligned}
 Y_{VW} &= \text{the volumetric heat dissipation admittance for the water-} \\
 &\quad \text{cooled portion of the fuel, H/}^\circ\text{T}, \\
 Y_{VG} &= \text{the volumetric heat dissipation admittance for the steam-} \\
 &\quad \text{cooled portion of the fuel, H/}^\circ\text{T}.
 \end{aligned}$$

Using Equation (2-75) and appropriate terms for S_{node} and Δx , the following equations may be written:

$$Y_{VW} = \frac{2(1-B) h_{FL} S_{\text{FUEL}} Z_W}{a} \tag{2-86}$$

and

$$Y_{VG} = \frac{2(1-B) h_{FV} S_{\text{FUEL}} (Z_1 - Z_W)}{a} \tag{2-87}$$

where

S_{FUEL} = the cross-sectional area of the fuel, L^2 .

After inserting the values of a , B and S_{FUEL} , these equations are rewritten as

$$Y_{VW} = 173 Z_W h_{FL} \quad (2-88)$$

and
$$Y_{VG} = 173 (Z_i - Z_W) h_{FV} \quad (2-89)$$

where Y_{VW} and Y_{VG} are in units of B/sec-°F.

The coefficients for heat transfer by natural convection from the water in the cavity to the inner surface of the cavity, and the coefficients for heat transfer to the steam in the outer jacket, from the surfaces bounding the water jacket, were obtained by the same procedures used to obtain h_{FL} and h_{FV} . These coefficients were obtained from the Colburn-Hougen equation for liquids and gases heated on vertical plates⁽¹⁵⁾ [see Equation (3-3) of Section 3.1.2]. The large diameter surfaces in the cask were assumed to behave the same as vertical plates. Stoever⁽¹⁵⁾ has also evaluated the Colburn-Hougen equation for several liquids and gases and presented the results as a base heat transfer coefficient as a function of the temperature difference between the surface and the coolant. These results are also plotted on log-log plots and may be represented by Equation (1-17).

Using the same procedure described above, the following equations were obtained for the heat transfer coefficients at the inner surface of the cask cavity:

$$h_L = 0.0089 (|T_W - T_C|)^{0.3355} \quad (2-90)$$

and
$$h_V = 1.25 \times 10^{-4} F_P (|T_W - T_C|)^{0.375} \quad (2-91)$$

where

- h_L = the coefficient for heat transfer by natural convection from the water in the cask to the inner surface of the cask cavity, B/sec-ft²-°F,
- h_V = the coefficient for heat transfer by natural convection from the steam in the cask to the inner surface of the cask cavity, B/sec-ft²-°F,
- T_C = the temperature of the inner surface of the cask cavity, °F
- F_P = the pressure correction factor applied to the base coefficient for steam
= $f(P)$. (2-92)

Like Y_V , the admittance for heat transfer by natural convection from the water-steam mixture to the inner surface of the cask cavity consists of a water portion and a steam portion

$$Y_1 = Y_{1V} + Y_{1L} \quad (2-93)$$

$$Y_1 = \pi D(Z_i - Z_W) h_V + \pi D Z_W h_L \quad (2-94)$$

$$= \pi D \left[(Z_i - Z_W) h_V + Z_W h_L \right] . \quad (2-95)$$

The heat transfer coefficients and admittances for natural convection of steam in the outer jacket are:

$$h_{JS} = 1.25 \times 10^{-4} (|T_J - T_{JC}|)^{0.375} \quad (2-96)$$

$$h_{SB} = 1.25 \times 10^{-4} (|T_{JC} - T_B|)^{0.375} \quad (2-97)$$

$$Y_5 = \pi D_J Z_i h_{JS} \quad (2-98)$$

$$Y_6 = \pi D_B Z_i h_{SB} \quad (2-99)$$

where

h_{JS} = the coefficient for heat transfer by natural convection from the outer surface of the cask wall to the steam in the jacket, B/sec-ft²-°F,

h_{SB} = the coefficient for heat transfer by natural convection from the steam in the jacket to the inside surface of the corrugated barrel, B/sec-ft²-°F,

Y_5 = the admittance corresponding to h_{JS} , B/sec-°F,

Y_6 = the admittance corresponding to h_{SB} , B/sec-°F,

D_J = the diameter of the outer cask wall, ft,

D_B = the diameter of the corrugated barrel, ft.

The coefficient for heat transfer by radiation between two surfaces is defined by

$$h_r = \frac{\sigma (T_1^4 - T_2^4)}{(t_1 - t_2)} \quad (2-100)$$

where

σ = the Stefan-Boltzmann constant, B/hr-ft²-°R⁴,

T_1 and T_2 = the absolute temperatures of the two surfaces, °R

t_1 and t_2 = the temperatures of the two surfaces, °F.

Stoever⁽¹⁶⁾ has evaluated this equation for temperatures from 0 to 2400°F and presented the results in the form of a chart. This chart was programmed into the model as the bivariate function

$$h_r = f(t_1, t_2) \quad (2-101)$$

with h_r in units of B/sec-ft²-°F and the temperatures in °F.

The admittance for heat transfer by radiation across the outer water jacket is derived from Equations (2-79) and (2-101), i.e.,

$$Y_3 = \pi D_J Z_i F h_{rJB} \quad (2-102)$$

where $h_{rJB} = f(T_J, T_B) \quad (2-103)$

and $F = F_A F_\epsilon \quad (2-104)$

The shape factor, F_A , is assumed to be 1.0, and the emissivity factor is assumed to be

$$F_\epsilon = \epsilon_J \epsilon_B \quad (2-105)$$

where

$$\epsilon_J = \begin{array}{l} \text{the emissivity of the outer surface of the cask wall} \\ \cong 0.8 \end{array}$$

$$\epsilon_B = \begin{array}{l} \text{the emissivity of the corrugated barrel} \\ \cong 0.8. \end{array}$$

Finally, the admittance for heat transfer by combined radiation and natural convection from the outer surface of the corrugated barrel was written as

$$Y_4 = \pi D_B Z_i (h_{Bo} + h_{ro}) \quad (2-106)$$

where

h_{Bo} = the coefficient for heat transfer by natural convection to air and steam at the outer barrel surface, $B/sec-ft^2-^{\circ}F$,

h_{ro} = the coefficient for heat transfer by radiation from the outer surface of the barrel to the surroundings, $B/sec-ft^2-^{\circ}F$.

The coefficient h_{Bo} is defined by the equation

$$h_{Bo} = 1.25 \times 10^{-4} (|T_B - T_S|)^{0.375} \quad (2-107)$$

and h_{ro} by the equation

$$h_{ro} = f(T_B, T_S) \quad (2-108)$$

where

T_S = the temperature of the surroundings, $^{\circ}F$.

Thermal capacities are defined by the general equation

$$C = \rho C_p V \quad (2-109)$$

where

C_p = the heat capacity of the region material, H/MT ,

ρ = the density of the material, M/L^3 ,

V = the volume of the region, L^3 .

Since the fuel is porous, its volume must be expressed as

$$V_F = (1-B) V_{FR} \quad (2-110)$$

where

V_{FR} = the overall volume of the fuel region of length Z_1 , L^3 .

The thermal capacity of the cask wall was computed as a volume-weighted average of the thermal capacities of steel and uranium.

The thermal capacity of the mixture of water and steam was assumed to be

$$C_{MIX} = C_{PG} \rho_G V + M_W \quad (2-111)$$

where

C_{PG} = the heat capacity of the steam, H/MT.

The heat generated in the fuel region is the maximum decay heat rate in the cask obtained from Table 1, converted to B/sec.

2.1.1.3.2 Energy Balance on the Fuel

An energy balance on the fuel region of Figure 2-4 is

$$C_F \frac{dT_F}{dt} = Q - Y_V (T_F - T_W) \quad (2-112)$$

where

C_F = the thermal capacity of the fuel region, H/T

Q = the decay heat generated in the fuel, H/θ.

2.1.1.3.3 Energy Balance on the Coolant

The energy balance on the coolant may be written as

$$C_{MIX} \frac{dT_W}{dt} = Y_V (T_F - T_W) - Y_1 (T_W - T_C) \quad (2-113)$$

2.1.1.3.4 Energy Balances on the Cask Wall

The energy balance on the inner half of the cask wall is

$$C_{C1} \frac{dT_C}{dt} = Y_1 (T_W - T_C) - Y_2 (T_C - T_J) \quad (2-114)$$

where

C_{C1} = the thermal capacity of the inner half of the cask wall, H/T.

The energy balance on the outer half of the cask wall is

$$C_{C2} \frac{dT_J}{dt} = Y_2 (T_C - T_J) - Y_3 (T_J - T_B) - Y_5 (T_J - T_{JC}) \quad (2-115)$$

where

C_{C2} = the thermal capacity of the outer half of the cask wall, H/T.

2.1.1.3.5 Energy Balance on the Outer Surface of the Water Jacket

The energy balance on the corrugated barrel or outer surface of the water jacket may be written as

$$C_B \frac{dT_B}{dt} = Y_3 (T_J - T_B) - Y_4 (T_B - T_S) + Y_6 (T_{JC} - T_B) \quad (2-116)$$

where

C_B = the thermal capacity of the barrel, H/T.

2.1.1.3.6 Energy Balance on the Steam in the Water Jacket

The energy balance on the residual steam in the water jacket may be expressed as

$$0 = Y_5 (T_J - T_{JC}) - Y_6 (T_{JC} - T_B) \quad (2-117)$$

or, in terms of the temperature of the steam,

$$T_{JC} = \frac{Y_5 T_J + Y_6 T_B}{Y_5 + Y_6} \quad (2-118)$$

It was assumed that heat storage in the residual vapor is negligible compared to that in the surrounding surfaces and that, for convenience, it could be neglected.

2.1.1.3.7 Determination of Temperatures From the Energy Balances

The temperatures of the various regions of the cask model are determined by integrating the energy balance equations, i.e.,

$$T_F = T_{Fi} + \int_0^t \frac{dT_F}{dt} dt \quad (2-119)$$

$$T_W = T_{Wi} + \int_0^t \frac{dT_W}{dt} dt \quad (2-120)$$

$$T_C = T_{Ci} + \int_0^t \frac{dT_C}{dt} dt \quad (2-121)$$

$$T_J = T_{Ji} + \int_0^t \frac{dT_J}{dt} dt \quad (2-122)$$

$$T_B = T_{Bi} + \int_0^t \frac{dT_B}{dt} dt \quad (2-123)$$

where T_{Fi} , T_{Wi} , T_{Ci} , T_{Ji} and T_{Bi} are the initial temperatures.

All the simulation models in Sections 2 and 4 include several equations which must be integrated with respect to time. Therefore, a brief discussion of the integrator statement used in MIMIC is appropriate at this time.

All integrations in the MIMIC simulation program are performed by a centralized integration routine. The particular algorithm employed is the fourth order variable step Runge-Kutta method.

The integrator statement is normally used with two inputs, an integrand A and an initial condition B. The integrator statement is written as

$$R = \text{INT} (A,B) \quad (2-124)$$

where R is the result of the integration. This statement is the equivalent of

$$R = B + \int_0^t A dt \quad (2-125)$$

where t is the time. There are three modes of operation for the integrators in MIMIC that can be controlled for each individual integrator. These modes of operation are RESET, OPERATE and HOLD. In RESET, the output of the integrator is set equal to the initial condition argument and no integration takes place. In OPERATE, the integrator is updated by the integration routine. In HOLD, the input to the integrator is removed. These modes are controlled by two additional arguments of the integration statement (see Figure 2-2),

$$R = \text{INT} (A,B,C,D). \quad (2-126)$$

The additional arguments C and D are either true or false, and the four possible combinations control the mode of each integrator, as shown in the following table.

D \ C	TRUE	FALSE
TRUE	OPERATE	HOLD
FALSE	RESET	OPERATE

If C and D are not specified, as in Equation (2-14), the integrator mode is automatically set at OPERATE. Mode-controlled integration is illustrated later in Section 2.2.2.3.2, where logical control variables are used to control the integrator mode.

The MIMIC integration statements equivalent to Equation (2-119) through (2-123) are

$$TF = \text{INT}(DTF, TFI) \quad (2-127)$$

$$TW = \text{INT}(DTW, TWI) \quad (2-128)$$

$$TC = \text{INT}(DTC, TCI) \quad (2-129)$$

$$TJ = \text{INT}(DTJ, TJI) \quad (2-130)$$

$$TB = \text{INT}(DTB, TBI). \quad (2-131)$$

where

$$DTF = \frac{dT_F}{dt}, \quad TFI = T_{Fi}, \text{ etc.}$$

The temperature of the vapor in the water jacket is obtained from Equation (2-118). However, a MIMIC "implicit function" must be used to avoid a closed algebraic loop. This algebraic loop is formed because T_{JC} is used to determine T_B and T_J , which are then used in Equation (2-118) to determine T_{JC} . The implicit function evaluates Equation (2-118) in an iterative manner. Equation (2-118), written in terms of the equivalent MIMIC implicit function statement, becomes

$$TJC = \text{IMP}(TJC, (Y5*TJ + Y6*TB)/(Y5 + Y6)) \quad (2-132)$$

where an initial or starting value of T_{JC} is entered as an input parameter. An implicit function was also required earlier, in Section 2.1.1.2, to overcome an algebraic loop involving the liquid column height, Z_w . See Reference 3 for a detailed discussion of the implicit function.

2.1.2 Coolant Loss From the Cask While in a Breach Up Position

When the cask is in a breach up position, only saturated vapor flows through the breach, and the potential energy of the liquid coolant is no longer part of the force driving coolant from the cask. Aside from a few changes required to simulate these new conditions, the coolant loss rate model for the cask in a breach up position is almost the same as the model developed in the previous section for the breach down position.

The changes required to convert the breach down version of the model into the breach up version are:

- (1) Since only saturated vapor flows through the breach, Equation (2-21) is changed to

$$Z = Z_p. \quad (2-133)$$

- (2) The logical control variable CNTRCT is removed as the control on Equations (2-72) and (2-73), which define the logical control variables CLNT and EMPTY, respectively.
- (3) XPAND replaces CLNT as the control variable on Equations (2-18), (2-25) and (2-29), and
- (4) CNTRCT replaces EMPTY as the control on Equations (2-64), (2-65) and (2-66).

A MIMIC listing of the breach up version of the coolant loss rate model is presented in Figure 2-5.

2.2 Rate of Coolant Loss From the AMCO Cask

Two separate and dissimilar coolant loss rate models were developed for the AMCO cask. The first model, the breach down model, is based on an energy balance relating the isentropic flow of Dowtherm-A through the breach to the potential energy of the coolant column. This model, developed in Section 2.2.1, is presented as a MIMIC listing in Figure 2-6.

```

*
IF CLR
*
*****BREACH DOWN *****
*
      CON(MWI,PI,VI,AGAP,TWI)
      CON(ZI,GC,PATM)
      CON(Q,MOLV,R)
      CON(J)
      CON(KHV,U,DJ, KHJS, DB)
      CON(CC1,CC2,CB,K,F,CPG)
      CON(TCI,TJI,TBI)
      CON(KHFV,TFI,CF)
      KHO      = CFN(4.)
      GMAX      = CFN(6.)
      GMAXV     = CFN(6.)
      HFG       = CFN(6.)
      FPF       = CFN(7.)
      TSF       = CFN(4.)
      HK        = CFN(16.)
      FPFVF     = CFN(7.)
      HWF       = CFN(6.)
      HGF       = CFN(6.)
      RHUV      = CFN(6.)
      PSAT      = CFN(11.)
      PAK(TJC)
      PAK(ZW)
      TEO      = FSW(T,TRUE,TRUE,FALSE)
      TGTU     = NOT(TEO)
      TEO      ACASK = MWI/(RHOW*ZI)
      KHOW      = FUN(KHO,TW )
      HVAP      = FUN(HFG,P)
      TEO      VCASK = ACASK*ZI
      CNTRCT    CLNT  = FSW(MW,FALSE,FALSE,TRUE)
      CNTRCT    EMPTY = NOT(CLNT)
      XPAND     P      = FUN(PSAT,TW)
      CNTRCT    P      = MV*R*(TW+460.)/(MOLV*V*144.)
      EMPTY     V      = VCASK
      CLNT      V      = MV/RHUG
      DTF       = (Q-YV*(TF-TW))/CF
      DTW       = (YV*(TF-TW)-Y1*(TW-TC))/CMIX
      DTC       = (Y1*(TW -TC)-Y2*(TC-TJ))/CC1
      DTJ       = (Y2*(TC-TJ)-Y3*(TJ-TB)-Y5*(TJ-TJC))/CC2
      DTB       = (Y3*(TJ-TB)-Y4*(TB-TS)+Y6*(TJ-TB))/CR
      TF        = INT(DTF,TFI)
      TW        = INT(DTW,TWI)
      TC        = INT(DTC,TC1)
      TJ        = INT(DTJ,TJI)
      TB        = INT(DTB,TBI)
      TS        = FUN(TSF,T)
      TJC       = IMP(TJC,(Y5*TJ+Y6*TB)/(Y5+Y6))
      CMIX      = CPG*RHOG*V+MW
      YV        = YVG+YVW
      YVW       = 173.*ZW * HFL
      YVG       = 173.*(ZI-ZW)*HFV
      HFL       = .0133*EXP(.25,ABS(TF-TW))
      HFV       = KHFV*FPFV*EXP(.256,ABS(TF-TW))
      FPFV      = FUN(FPFV,P)
      RHOG      = FUN(RHUV,TW)

```

FIGURE 2-5. MIMIC Listing of the Coolant Loss Rate Model of the IF-300
 (Breach Up Version) (Page 1 of 3)

```

Y1      = 3.14*D*((Z1-ZW)*HV+ZW*HL)
HL      = .0089*EXP(.3355,ABS(TW -TC))
HV      = KHV*FP*EXP(.375,ABS(TW -TC))
FP      = FUN(FPF,P)
Y2      = 3.14*(D+DJ)*Z1*K/(DJ-D)
Y3      = 3.14*F*DJ*Z1*HRJB
HRJB    = FUN(HR,TJ,TB)
Y5      = 3.14*DJ*Z1*HJS
HJS     = KHJS*EXP(.375,ABS(TJ-TJC))
Y6      = 3.14*DB*Z1*HSB
HSB     = KHJS*EXP(.375,ABS(TJC-TB))
Y4      = 3.14*DB*Z1*(HBO+HRO)
HBO     = KHJS*EXP(.375,ABS(TB-TS))
HRO     = FUN(HR,TB,TS)
RHOX    = MX/VCASK
XOFF    = FSW(ZW-14.,FALSE,TRUE,TRUE)
XON     = NOT(XOFF)
XOFF    X      = 0.
XON     QUALTY = (1./RHOX-1./RHOW)/(1./RHOG-1./RHOW)
XON     X      = LIM(QUALTY,0.,1.)
DMX     = -GOUT*AGAP/144.
MX      = INT(DMX,MWI)
MWU     = MWI-MX
MV      = X*MX
MW      = (1.-X)*MX
QGRAD   = Y1*(TW-TC)
QOUT    = QGRAD
QIN     = YV*(TF-TW)
QNET    = QIN-QOUT
GMAXG   = FUN(GMAXV,P)
GMAXF   = FUN(GMAX,P)
XPAND   = FSW(X,TRUE,TRUE,FALSE)
CNTRCT  = NOT(XPAND)
XPAND   G      = RHOW*SQR(2.*GC*Z)
XPAND   GOUT   = MIN(G,GMAXF)
CNTRCT  G      = RHOG*SQR(2.*GC*Z)
CNTRCT  GOUT   = MIN(G,GMAXG)
Z       = ZP
ZWA     = LIM(MW/(RHOW*ACASK),0.,14.)
ZW      = IMP(ZW,ZWA)
XPAND   ZP     = (P-PATM)*144./RHOW
CNTRCT  ZP     = (P-PATM)*144./RHOG
DTMAX   = 5.0
UT      = 60.
HOURS   = T/3600.
        FIN(PATM,P)
        FIN(T,43200.)
        OUT(T,MW,MWU,GMAXF,G,GOUT)
        OUT(HOURS,ZP,ZW,Z,MV,X)
        OUT( ,MX,HVAP,MVT,GMAXG)
        OUT( ,P,V,V0)
        OUT( ,ZC,QUALTY)
        OUT( ,RHOW,RHOG, RHOX)
TEO      OUT( ,MWI,VCASK,ACASK)
        OUT( ,QGAP,QGRAD,QIN)
        OUT( ,QOUT,QNET)
        OUT( ,TF,TW, CMIX, CPG)
        OUT( ,TC,TJ,TB,TS,TJC)
        OUT( ,YV,YVW,YVG)
        OUT( ,Y1,Y2,Y3, Y5, Y6)
        OUT( ,Y4,HL,HV,FP,HJS)
        OUT( ,HFL,HFW,FPFV,HW,HG)
        OUT( ,HSB,HBO,HRJB,HRO)

```

FIGURE 2-5. MIMIC Listing of the Coolant Loss Rate Model of the IF-300 (Breach Up Version) (Page 2 of 3)

```

OUT
PLU(T,TF,TW,TC,TJ, TH)
PLU(T,TJC,TS)
PLO(T,MW,MWO,ZW,P,X)
PLO(T,MX)
PLU(T,GMAXF,G,GOUT,GMAXG)
END

```

FIGURE 2-5. MIMIC Listing of the Coolant Loss Rate Model of the IF-300
(Breach Up Version) (Page 3 of 3)

The second model, the breach up model, is primarily a transient heat transfer simulation of the cask in which energy balances are used to determine the time required to bring the Dowtherm-A to its saturation temperature, and the time required to lose the coolant due to vaporization. This model, developed in Section 2.2.2, is presented as a MIMIC listing in Figure 2-9.

2.2.1 Coolant Loss From the Cask While in a Breach Down Position

The average temperature of the Dowtherm-A in the cask, as determined by the steady-state pre-accident model, is about 360°F. The saturation pressure at this temperature is about 2.0 psia, well below atmospheric pressure. This means that the Dowtherm is subcooled.

When the Dowtherm-A is subcooled, and the cask lands with the breach down, the only force driving the coolant from the cask would be the potential energy of the coolant column. The static pressure in the cask would not be a factor, since it would not be greater than the atmospheric pressure.

A MIMIC listing of the breach down version of the coolant loss rate model of the AMCO cask is presented in Figure 2-6.

2.2.1.1 Energy Balance on the Breach

The energy balance on the breach would be the same as the energy balance developed earlier in Section 2.1.1.1 for the IF-300, except that the pressure energy or flow work term

$$vdP = 0 . \quad (2-134)$$

The final equation in Section 2.1.1.1, which defines the mass velocity of the coolant leaving the cask, would be the same

$$G = \rho_w \sqrt{2g_c Z} , \quad (2-25)$$

but now

$$Z = Z_w \quad (2-135)$$

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```

AGCLR  **  *SUBROUTINE DOU  *  **
      CON(MWI,GC,ZI,TW,AGAP)
      RHO  = JFN(5.)
      TEO  = FSW(T,TRUE,TRUE,FALSE)
      ACASK = MWI/(RHOW*Z1)
      MW   = MWI-MWO
      MWO  = INT(GMAX*AGAP/144.,0.)
      Z    = MW/(RHOW*ACASK)
      TEO  = FUN(RHO,TW)
      GMAX = RHOW*SQR(2.*GC*Z)
      DT   = 100.
      HOURS = T/3600.
      FIN(MWO,3790.)
      FIN(T,32400.)
      OUT(T,MW,MWO)
      OUT(HOURS,Z,GMAX)
      OUT( ,RHOW,ACASK)
      OUT
      OUT
      PLO(T,MW,MWO)
      PLO(T,Z,GMAX)
      END
  
```

FIGURE 2-6. MIMIC Listing of the Coolant Loss Rate Model of the AMCO Cask (Breach Down Version)

instead of

$$Z = Z_W + Z_p, \quad (2-21)$$

since

$$\begin{aligned} Z_p &= \frac{P - P_{ATM}}{\rho_W} \\ &= 0. \end{aligned} \quad (2-18)$$

2.2.1.2 Rate of Coolant Loss From the Breach and Mass Balance on the Cask

When the cask is in a breach down position, only the subcooled Dowtherm-A would flow through the breach. The maximum mass velocity of the coolant flowing from the breach would be the same as the mass velocity defined by Equation (2-25), i.e.,

$$G_{MAX} = G = \rho_W \sqrt{2g_c Z}, \quad (2-136)$$

where

$$Z = Z_W = \frac{M_W}{\rho_W A_{CASK}} \quad (2-137)$$

and

$$A_{CASK} = \frac{M_{wi}}{\rho_W Z_i}. \quad (2-20)$$

The rate at which coolant is lost from the breach is

$$\frac{dM_{wo}}{dt} = G_{MAX} A_{GAP} \quad (2-138)$$

where

A_{GAP} = the flow area of the breach, L^2 .

The total mass of coolant lost at any time is

$$M_{wo} = \int_0^t G_{MAX} A_{GAP} dt + M_{woi} \quad (2-139)$$

where

M_{wo} = the mass of coolant lost, M

M_{woi} = the initial mass of coolant lost, M
= 0 .

Finally, a mass balance on the cask may be written as

$$M_w = M_{wi} - M_{wo} \quad (2-140)$$

where

M_w = the mass of coolant remaining in the cask, M

M_{wi} = the mass of coolant initially in the cask, M.

2.2.2 Coolant Loss From the Cask While in a Breach Up Position

The coolant loss rate model developed in this section is primarily a transient heat transfer simulation of the AMCO cask. Energy balances are used to determine the time required to bring the Dowtherm-A to its saturation temperature, and the time required to lose the coolant by vaporization. An idealized model of the cask, in the form of an electrical analog, is shown in Figure 2-7. This idealized cask consists of five components or regions for which energy balances were written to form the model. These regions are:

1. the fuel assemblies, represented as one homogeneous region,
2. a basket region surrounding the fuel region,
3. the coolant,

HEDL 7507-30.6

FIGURE 2-7. Idealized Representation of the AMCO Cask as an Electrical Analog

4. the cask wall, represented as one region, including the outer cooling jacket, and
5. the outer surface of the cask wall.

Only coolant vapor would be lost from the cask when it is in a breach up position. At the time of the accident, it was assumed that the cask loses its solar shield and all of the water in its outer jacket or neutron shield. The loss of the water in the outer jacket creates a barrier in the path of the heat flowing from the cask, consequently the temperatures in the cask gradually increase. Also, loss of the solar shield allows an increase in the heat input to the cask at its outer surface. As the temperatures in the cask increase, the Dowtherm-A reaches its saturation temperature and vapor is formed.

Energy balances that describe the thermal behavior of the cask before the coolant reaches saturation conditions are presented in Section 2.2.2.1. Modifications to this system of equations, which are required to simulate the thermal behavior of the cask during vaporization, are presented in Section 2.2.2.2.

The equations that form the model are presented in an algorithm or calculation flow diagram in Figure 2-8. A listing of the equations programmed for the MIMIC simulation code is presented as Figure 2-9.

Heat enters the cask in three forms:

1. as decay heat generated in the fuel,
2. as solar heat, and
3. as heat input from the fire.

Heat leaves the cask by natural convection and radiation from the cask surface to the surroundings, and in the coolant lost from the cask due to vaporization.

The initial temperatures in the cask are obtained from the temperature distribution established by the steady-state pre-accident model.

HEDL 7507-30.31

FIGURE 2-8. Calculation Control Flow Diagram of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 1 of 5)

HEDL 7507-30.32

FIGURE 2-8. Calculation Control Flow Diagram of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 2 of 5)

HEDL 7507-30.33

FIGURE 2-8. Calculation Control Flow Diagram of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 3 of 5)

HEDL 7507-30.34

FIGURE 2-8. Calculation Control Flow Diagram of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 4 of 5)

HEDL 7507-30.35

FIGURE 2-8. Calculation Control Flow Diagram of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 5 of 5)

A MODEL SIMULATING THE TRANSIENT BEHAVIOR OF THE AMCO SPENT FUEL SHIPPING CASK FOLLOWING AN ACCIDENT AND FIRE, WITH GRADUAL LOSS OF PRIMARY COOLANT (BREACH UP VERSION).

***** THIS MODEL IS PROGRAMMED IN A LANGUAGE FOR MIMIC, A CONTINUOUS SYSTEM SIMULATION PROGRAM *****

- (1) DOWTHERM-A COOLANT NOT LOST
- (2) PETROLEUM FIRE AT 1475 DEG F
- (3) ADMITTANCE FOR HEAT INPUT FROM FIRE FROM STEADY STATE CASE
- (4) HEAT BALANCES ON FUEL, SHROUDS, BASKETS, CANISTER, AND CASK
- (5) SOLAR INPUT INCLUDED
- (6) JACKET WATER LOST

NOMENCLATURE OF TERMS *****

AGAP = FLOW AREA OF THE BREACH OPENED IN THE CASK AT IMPACT, IN**2
 AOPENJ = FLOW AREA OF THE BREACH ASSUMED OPENED IN THE CASK AT IMPACT, IN**2 (J=1...5)
 CH = THERMAL CAPACITY OF THE BASKETS, B/DEGF
 CC = THERMAL CAPACITY OF CASK WALL, B/DEGF
 CF = THERMAL CAPACITY OF FUEL, B/DEGF
 CW = THERMAL CAPACITY OF THE COOLANT, B/DEGF
 DAYLIM = TIME LIMIT ON SIMULATION, DAYS
 DAYS = ELAPSED TIME OF SIMULATION, DAYS
 DMW = TIME DERIVATIVE OF MW, LBS/SEC
 DT = TIME STEP FOR PRINTOUT, SECONDS
 DTH = TIME DERIVATIVE OF TH, DEGF/SEC
 DTC = TIME DERIVATIVE OF TC, DEGF/SEC
 DTF = TIME DERIVATIVE OF TF, DEGF/SEC
 DTW = TIME DERIVATIVE OF TW, DEGF/SEC
 F = ARRAY NAME, FIRE TEMPERATURE AS A FUNCTION OF TIME.
 FIRE = LOGICAL CONTROL VARIABLE (LCV), LOGICAL COMPLEMENT OF NOFIRE TRUE OR ON WHEN T.LT.1800.SECONDS, OFF OTHERWISE.
 GGAP = MASS FLOW RATE OF PRIMARY COOLANT THROUGH AGAP, LB/SEC*FT**2
 GOPENJ = MASS FLOW RATE OF PRIMARY COOLANT THROUGH AOPENJ (J=1...5), LB/SEC*FT**2
 HOURS = ELAPSED TIME OF SIMULATION, HOURS
 HV = LATENT HEAT OF VAPORIZATION OF PRIMARY COOLANT, B/LB
 MW = MASS OF PRIMARY COOLANT REMAINING IN CASK, LBS
 MWI = AMOUNT OF PRIMARY COOLANT INITIALLY IN CASK, LB
 NOFIRE = LOGICAL CONTROL VARIABLE (LCV), FUNCTION SWITCH, TRUE OR ON WHEN T.GT.1800.SECONDS, OFF OTHERWISE.

FIGURE 2-9. MIMIC Listing of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 1 of 6)

QH = HEAT STORED IN BASKETS, B/SEC
 QC = HEAT STORED IN CASK WALL, B/SEC
 QF = HEAT STORED IN FUEL, B/SEC
 QW = HEAT REQUIRED TO VAPORIZE COOLANT, B/SEC
 QSOL = TOTAL SOLAR HEAT INPUT TO CASK SURFACE (FINS AND OUTER SHELL), B/SEC (QSOL=QSOLF IN DAYTIME, QSOL=0. AT NIGHT)
 QSOLF = TOTAL SOLAR HEAT INPUT TO THE CASK SURFACE (FINS AND OUTER SHELL) DURING 12 HOURS OF DAYLIGHT ON SUNNY DAY, B/SEC (USED 1/3 THE MAXIMUM HORIZONTAL ON SUNNY SIDE AS AVERAGE FOR ENTIRE SURFACE OF CASK)
 QSOLV = DIURNAL SOLAR HEATING FACTOR OF EITHER 1. OR 0., DEPENDING ON 12-HOUR TIME PERIOD.
 QVF = DECAY HEAT GENERATION IN FUEL ASSEMBLIES, B/SEC
 QW = HEAT STORED IN COOLANT, B/SEC
 QYB = HEAT TRANSFERRED FROM BASKETS TO COOLANT, B/SEC
 QYC1 = HEAT TRANSFERRED FROM CASK WALL INTERIOR TO OUTER CASK WALL, B/SEC
 QYC2 = HEAT TRANSFERRED FROM CASK WALL INTERIOR TO COOLANT, B/SEC
 QYCS = HEAT TRANSFERRED FROM CASK SURFACE TO SURROUNDINGS, B/SEC
 QYV = HEAT TRANSFERRED FROM FUEL ASSEMBLIES TO COOLANT, B/SEC
 WATEN = RATE OF LOSS OF PRIMARY COOLANT, LBS*IN**2/SEC*FT**2
 SOLQ = ARRAY NAME, DIURNAL HEATING FACTOR AS A FUNCTION OF TIME. (FACTOR= 0. DURING 12 HOURS OF DARKNESS AND FACTOR=1 DURING 12 HOURS OF SUNNY DAYLIGHT.)
 T = ELAPSED TIME OF SIMULATION, SECONDS
 TB = BASKET TEMPERATURE, DEGF
 TB1 = INITIAL BASKET TEMPERATURE AT IMPACT, DEGF
 TC = CASK WALL TEMPERATURE, DEGF
 TC1 = INITIAL CASK WALL TEMPERATURE AT IMPACT, DEGF
 TCS = CASK SURFACE TEMPERATURE, DEGF
 TCS1 = INITIAL CASK SURFACE TEMPERATURE AT IMPACT, DEGF
 TEO = LOGICAL CONTROL VARIABLE (LCV), FUNCTION SWITCH, TRUE OR ON WHEN T.LE.0, OFF OTHERWISE.
 TF = FUEL TEMPERATURE, DEGF
 TFR = FUEL TEMPERATURE, DEGF
 TGETS = LOGICAL CONTROL VARIABLE (LCV), FUNCTION SWITCH, TRUE OR ON WHEN TW.GE.TVS, OFF OTHERWISE.
 TGTO = LOGICAL CONTROL VARIABLE (LCV), LOGICAL COMPLEMENT OF TEO. ON IF T.GT.0, OFF OTHERWISE.
 TLTS = LOGICAL CONTROL VARIABLE (LCV), LOGICAL COMPLEMENT OF TGETS. TRUE OR ON WHEN TW.LT.TVS, OFF OTHERWISE.
 TW = COOLANT TEMPERATURE, DEGF
 TW1 = INITIAL COOLANT TEMPERATURE AT IMPACT, DEGF
 TF1 = INITIAL FUEL TEMPERATURE AT IMPACT, DEGF
 TWS = SATURATION TEMPERATURE OF PRIMARY COOLANT, DEGF
 YH = ADMITTANCE (Y) FOR HEAT TRANSFER (HT) BETWEEN BASKETS AND COOLANT, B/SEC*DEGF
 YC1 = Y FOR HT BETWEEN CASK WALL INTERIOR AND OUTER CASK WALL SURFACE, B/SEC*DEGF

FIGURE 2-9. MIMIC Listing of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 2 of 6)

```

.   YC2 = Y FOR HT BETWEEN CASK WALL INTERIOR AND COOLANT, R/SEC*DEGF
.   YC3 = Y FOR HT BETWEEN CASK SURFACE AND SURROUNDINGS, R/SEC*DEGF
.   YV = VOLUMETRIC HEAT DISSIPATION ADMITTANCE FOR HEAT TRANSFER
.       FROM FUEL ASSEMBLIES TO PRIMARY COOLANT, R/SEC*DEGF
.
.
.   SOLU      CFN(60.)
.   F          CFN(5.)
.              PAR(YV,YR,(F,CH,CW,TNS)
.              PAR(QVF,CC,YC1,YC2,GSOLF)
.              PAR(HV,MWI,YC3,DAYLIM)
.              PAR(TF1,TR1,TW1,TC1,TCS1)
.              PAR( AOPEN1,AOPEN2,AOPEN3,AOPEN4,AOPEN5)
.
.
.   COMPUTE DIURNAL SOLAR INPUT
.
.       QSOLV      FUN(SOLG,T)
.       QSOL       QSOLF * QSOLV
.
.   FIRE TEMP. VARIES WITH TIME
.
.       TFR        FUN(F,T)
.
.   FUNCTION SWITCH TEO. ON IF T.LE.0. OFF OTHERWISE.
.
.       TEO        FSW(T,TRUE,TRUE,FALSE)
.
.   LOGICAL CONTROL VARIABLE TGTO. ON IF T.GT.0. OFF OTHERWISE.
.   LOGICAL COMPLEMENT OF TEO)
.
.       TGTO       NOT(TEO)
.
.   FUNCTION SWITCH TGTS. ON IF TW.GE.TWS. OFF OTHERWISE.
.
.       TGTS       FSW(TW-TWS,FALSE,TRUE,TRUE)
.
.   LOGICAL CONTROL VARIABLE TLTS. ON IF TW.LT.TWS. OFF OTHERWISE.
.   (LOGICAL COMPLEMENT OF TGTS)
.
.       TLTS       NOT(TGTS)
.
.   COMPUTE FUEL TEMPERATURE
.
.       DTF        (QVF-YV*(TF-TW))/CF
.       TF         INT(DTF,TF1)
.

```

FIGURE 2-9. MIMIC Listing of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 3 of 6)

```

COMPUTE SENSIBLE HEAT TO DOW-A AND DOW-A TEMPERATURE
.
      CW      MW * .54
TLTTS  DTW    (YV*(TF-TW)-YH*(TW-TH)-YC2*(TW-TC))/CW
      TW      INT(DTW,TW1,TLTTS,TRUE)
.
COMPUTE RATE OF COOLANT LOSS AND AMOUNT OF COOLANT REMAINING
.
      TLTTS  DMW  = 0.
      TGETS  DMW  = -(YV*(TF-TW)-YH*(TW-TH)-YC2*(TW-TC))/HV
      MW      = INT(DMW,MW1,TGETS)
.
COMPUTE BASKET TEMPERATURE
.
      DTH      (YH*(TW-TH))/CH
      TH      INT(DTH,TH1)
.
COMPUTE CASK WALL TEMPERATURE
.
      DTC      (YC1*(TCS-TC)+YC2*(TW-TC))/CC
      TC      INT(DTC,TC1)
.
COMPUTE CASK WALL SURFACE TEMPERATURE
      TEO      TCS      EQL(TCS1)
      TGT0      TCS      (QSOL+YCS*TFH+YC1*TC)/(YCS+YC1)
.
COMPUTE HEAT FLOWS
.
      QYV      = YV*(TF-TW)
      QYH      = YH*(TW-TH)
      QYC2      = YC2*(TW-TC)
      QYCS      = YCS*(TCS-TFH)
      QYC1      = YC1*(TC-TCS)
      QH      = CH*DTH
      QF      = CF*DTF
      QC      = CC*DTC
      TLTTS  QW      = CW*DTW
      TGETS  QMW     = HV*DMW
.
COMPUTE MASS FLOW RATE OF PRIMARY COOLANT FROM CASK
.
      TGETS  RATEW  = (ABS(QMW)*144.)
      TGETS  GAP    = RATEW/AGAP
      TGETS  GOPEN1  = RATEW/AGOPEN1
      TGETS  GOPEN2  = RATEW/AGOPEN2
      TGETS  GOPEN3  = RATEW/AGOPEN3
      TGETS  GOPEN4  = RATEW/AGOPEN4
      TGETS  GOPEN5  = RATEW/AGOPEN5

```

FIGURE 2-9. MIMIC Listing of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 4 of 6)

```

TLTTS    GCRP    = 0.
TLTTS    GOPEN1 = 0.
TLTTS    GOPEN2 = 0.
TLTTS    GOPEN3 = 0.
TLTTS    GOPEN4 = 0.
TLTTS    GOPEN5 = 0.
.
COMPUTE TIME IN HOURS
.
      HOURS    = T/3600.
.
COMPUTE TIME IN DAYS
.
      DAYS     = HOURS/24.
.
STOP RUN WHEN MW=0. ALL DOWN-A VAPORIZED
.
      TGTTS          FIN(1.,MW)
.
STOP SIMULATION WHEN DAYS.GE.DAYLIM
.
      FJN(DAYS,DAYLIM)
.
TIME STEP FOR PRINTOUT= DT SEC
.
FUNCTION SWITCH NOFIRE.  ON IF TIME.GT.1800.SECONDS, OFF OTHERWISE.
.
      NOFIRE = FSW(T-1800.,FALSE,FALSE,TRUE)
.
LOGICAL CONTROL VARIABLE FIRE.  ON IF TIME.LE.1800.SECONDS,OFF OTHERWISE
(LOGICAL COMPLEMENT OF NOFIRE)
.
      FIRE    = NOT(NOFIRE)
.
TIME STEP FOR PRINTOUT
.
      FIRE     DT      = 300.
      NOFIRE    DT      = 7200.
.
.
OUTPUT
.
.
      OUT(T,TF,TR,TW,TC,TCS)
      OUT(HOURS,MW,QSOL,TFR)
      OUT(DAYS,QYV,QYF,QYC2,QYC1,QYCS)
      OUT( ,QSOL,QF,QH,QW,QC)
      OUT( ,OMW)

```

FIGURE 2-9. MIMIC Listing of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 5 of 6)


```

OUT ( .,SGAP,GOOPEN1,GOOPEN2,GOOPEN3,GOOPEN4)
OUT ( .,GOOPEN5)
OUT
OUT
PLO (H00F5,TF,TR,TW,TC,TCS)
SCA (5000.,.,.,.,.,.,.,.)
ZER (0.,-20.,-20.,-20.,-20.,-20.,)
END

```

FIGURE 2-9. MIMIC Listing of the Coolant Loss Rate Model of the AMCO Cask (Breach Up Version) (Page 6 of 6)

When the solar shield is lost, the cask is exposed to solar heating. A diurnal variation of the solar heat input was used in the model developed in this section and in the loss-of-coolant models discussed later in Section 3. It was assumed that the accident occurs at 6:00 a.m., and the solar heat falls on the cask at a constant rate until 6:00 p.m., when it drops to zero. This variation of solar heating was programmed into the models as a pulsed function of time, where this "on-off" characteristic was repeated as long as required. The solar heat reaching the cask was arbitrarily assumed to be one-third of that which would fall on a flat surface. This was an assumed correction factor to allow for the non-flat, 360°F cylindrical surface of a cask. It is impossible for the entire surface of a cask to face the sun.

The temperature of the surroundings is a function of time. During the fire, it is the temperature of the fire and, when the fire burns out, it becomes the ambient temperature of the surroundings. This variation of the temperature of the surroundings is programmed into the model as a time-varying step function.

2.2.2.1 Energy Balances in the Cask Before Vaporization of the Coolant

It is convenient to define and discuss in general, beforehand, some of the terms which will be used in the energy balance equations presented here and in Section 2.2.2.2.

Since the purpose of this model was to provide estimates of the time required for the cask to lose its coolant by vaporization, no attempt was made to determine detailed temperature distributions in the fuel, baskets and cask wall. Consequently, all of the thermal admittances in the heat balance equations are for heat transfer by combined conduction and convection or by combined conduction, convection and radiation. Each of the regions considered was represented as a single node.

All admittances, except the one representing heat transfer to the coolant from the fuel, are defined by the general equation

$$Y_h = UA \quad (2-141)$$

where

Y_h = the admittance for heat transfer by combined conduction and convection or by combined conduction, convection and radiation, $H/\theta T$,

U = an overall coefficient for heat transfer, $H/\theta LT$,

A = the area for heat transfer, L^2 .

The heat transfer submodel of the coolant loss rate model of the IF-300, developed in Section 2.1.1.3, was developed after the model discussed here and, consequently, includes some significant improvements. Some of these are related to the calculation of the heat transfer admittances. First of all, individual admittances were used for conduction, convection and radiation paths rather than admittances based on combinations of paths. Second, equations for the heat transfer coefficients for convection and radiation were included in the IF-300 model and were evaluated as functions of the temperatures. For the AMCO cask, temperatures were estimated beforehand, the heat transfer coefficients determined from side calculations, and these were then used to determine the appropriate admittances. The admittances then remained constant throughout the transient. Any future work on the AMCO cask model should include revisions of the network and computational procedure to match those used for the IF-300 model.

Heat transfer by natural convection from the fuel to the coolant was represented by a volumetric heat dissipation admittance defined by Equation (1-15) in Section 1.2., i.e.,

$$Y_v = \frac{2(1-B)h S_{node} \Delta x}{a} \quad (2-142)$$

where

Y_v = the volumetric heat dissipation admittance, $H/\theta T$,

B = the void fraction of the fuel region,

- h = the coefficient for heat transfer by natural convection from a fuel pin to the coolant, $H/\theta L^2 T$,
 a = the fuel pin radius, L ,
 S_{node} = the cross sectional area of a fuel node (in this case, S_{node} is the cross sectional area of the entire fuel region), L^2 ,
 Δx = the incremental length of the fuel region (in this case, Δx represents the lengths of the respective vapor-and-liquid-cooled portions of the fuel), L .

The coefficient for heat transfer by natural convection from a fuel pin to the coolant was obtained using the following correlation⁽²⁾

$$\frac{hD}{k} = 0.53 \left(\frac{D^3 \rho^2 g \beta \Delta T C_p}{\mu k} \right)^{1/3} \quad (2-143)$$

where

- h = the heat transfer coefficient, $H/L^2 \theta T$,
 D = the fuel pin diameter, L
 k = thermal conductivity of the coolant, $H/L \theta T$,
 ρ = coolant density, M/L^3
 g = gravitational constant, $ML/F \theta^2$,
 β = volume expansion coefficient of the coolant, $1/T$
 ΔT = the temperature difference between the coolant and the fuel pin, T ,
 C_p = the heat capacity of the coolant, H/MT ,
 μ = the viscosity of the coolant, $M/L \theta$.

This same correlation was used to obtain the coefficient for heat transfer from the coolant to the inside surface of the cask cavity, and between the basket and the coolant.

The admittance for heat transfer from the interior of the cask wall to the outer shell of the outer jacket, Y_{C1} , (see Figure 2-7) includes a complex network of conduction, convection and radiation paths from the outer

surface of the cask wall, through the fins and empty water jacket, to the outer surface of the cask (the outer shell of the water jacket, and the protruding portion of the fins). The network representing the empty water jacket of the AMCO cask is shown in Figure 3-21. The admittances in the network of Figure 3-21 were combined into one equivalent admittance, using network reduction methods. As stated earlier, the loss-of-coolant models were developed before the coolant loss rate models, so the conduction, convection and radiation admittances in the network had already been determined. The conduction and convection admittances had been predetermined, and the radiation admittances were determined by the TAP code during the course of the loss-of-coolant transient (see Section 3.4.1).

Thermal capacities are defined by the general equation

$$C = \rho C_p V \quad (2-144)$$

where

$$\begin{aligned} C_p &= \text{the heat capacity of the region material, H/MT,} \\ \rho &= \text{the density of the material, M/L}^3, \\ V &= \text{the volume of the region, L}^3. \end{aligned}$$

Since the fuel region is porous, its volume must be expressed as

$$V = (1-B) V_{FR} \quad (2-145)$$

where

$$\begin{aligned} V_{FR} &= \text{the overall volume of the fuel region, L}^3, \\ B &= \text{the void fraction.} \end{aligned}$$

The heat generated in the fuel region is the total thermal power in kilowatts obtained from Table 3, converted to B/sec.

2.2.2.1.1 Energy Balance on the Fuel

The energy balance on the fuel region of Figure 2-7 is

$$C_F \frac{dT_F}{dt} = Q_{VF} - Y_V (T_F - T_w) \quad (2-146)$$

where

C_F = the thermal capacity of the fuel region, H/T,

T_F = the temperature of the fuel region, T,

Q_{VF} = the decay heat generated in the fuel, H/θ,

Y_V = the volumetric heat dissipation admittance for the transfer of heat by convection from the fuel region to the coolant, H/θT,

T_w = the temperature of the coolant, T.

2.2.2.1.2 Energy Balance on the Basket

The energy balance on the basket region may be written as

$$C_B \frac{dT_B}{dt} = Y_B (T_w - T_B) \quad (2-147)$$

where

C_B = the thermal capacity of the basket, H/T,

T_B = the temperature of the basket region, T,

Y_B = the admittance for the transfer of heat by convection from the basket region to the coolant, H/θT.

The heat transfer area used in the admittance Y_B is the combined areas of the inner and outer surfaces of the basket.

2.2.2.1.3 Energy Balance on the Cask Wall

The energy balance on the cask wall is

$$C_C \frac{dT_C}{dt} = Y_{C1} (T_{CS} - T_C) + Y_{C2} (T_w - T_C) \quad (2-148)$$

where

C_C = the thermal capacity of the cask wall, H/T,

T_C = the temperature of the cask wall, T,

Y_{C1} = the equivalent admittance for heat transfer by combined conduction, convection and radiation from the interior of the cask wall, through the empty water jacket, to the outer shell of the water jacket, H/°T,

T_{CS} = the temperature of the outer surface of the cask (the outer shell of the water jacket and the protruding fins), T,

Y_{C2} = the equivalent admittance for the combined transfer of heat by convection from the primary coolant to the inner surface of the cask wall, and by conduction from the surface to the cask wall interior, H/°T.

2.2.2.1.4 Energy Balance on the Coolant

The energy balance on the coolant before it reaches its saturation temperature is

$$C_W \frac{dT_W}{dt} = Y_V(T_F - T_W) - Y_B(T_W - T_B) - Y_{C2}(T_W - T_C) \quad (2-149)$$

where C_W = the thermal capacity of the Dowtherm-A coolant, H/T.

Equation (2-149) is valid as long as the temperature of the Dowtherm-A is less than its saturation temperature. A different equation, presented in Section 2.2.2.2, is used when the coolant reaches saturation conditions. The procedure used to switch equations in the model at the proper time will also be described in Section 2.2.2.2.

2.2.2.1.5 Energy Balance at the Cask Surface

The electrical analog of the idealized model of the cask, Figure 2-7, does not include a thermal capacity for the node representing the cask surface. This means that, although heat is stored in the thin outer shell

and the fins, it was considered to be small enough compared to the thermal capacity of the cask wall that, for convenience, it could be neglected. This is believed to be a conservative assumption since there would now be no lag in the response of the surface to the heat input from the fire and solar heating, and no delay in transmitting this heat to the cask wall.

The energy balance at the cask surface may be written as

$$0 = Q_{SOL} + Y_{C1} (T_C - T_{CS}) - Y_{CS} (T_{CS} - T_{FR}) . \quad (2-150)$$

Rearrangement of Equation (2-150) gives the temperature of the cask surface as

$$T_{CS} = \frac{Q_{SOL} + Y_{C1} T_C + Y_{CS} T_{FR}}{Y_{C1} + Y_{CS}} \quad (2-151)$$

where

Q_{SOL} = the solar heat input, H/θ ,

Y_{CS} = the admittance for heat transfer by convection and radiation between the surroundings and the cask surface (water jacket outer shell and fins), $H/\theta T$,

T_{FR} = the temperature of the surroundings, either the fire or ambient conditions, T .

The temperature of the surroundings, T_{FR} , is a function of time. During the fire, it is the temperature of the fire and, when the fire burns out, it becomes the ambient temperature of the surroundings. This variation of the temperature of the surroundings is programmed into the model as a time-varying step function.

The solar heat input is also a function of time. During the 12 hours of daylight, solar heat is added to the cask at a rate of 19.5 B/sec. During the 12 hours of darkness, there is no solar heat input. This diurnal variation of solar heating is programmed into the model as an oscillating function of time, as shown in Figures 15 and 16.

2.2.2.2 Energy Balances in the Cask During Vaporization of the Coolant

When the Dowtherm-A coolant reaches saturation conditions, it boils, and the vapor formed flows through the breach opened in the cask containment at impact. For this case, all the energy balances presented in Section 2.2.2.1 remain the same, except for the energy balance on the coolant.

The energy balance on the coolant, when it reaches saturation conditions, is

$$- H_v \frac{dM_w}{dt} = Y_v(T_F - T_w) - Y_B(T_w - T_B) - Y_{C2}(T_w - T_C) \quad (2-152)$$

where

H_v = the latent heat of vaporization of the Dowtherm-A at the saturation temperature T_{ws} , H/M,

$\frac{dM_w}{dt}$ = the rate of change of the mass of coolant in the cask, M/ θ ,

T_w = the saturation temperature, T.

At this point, the temperature is held at the saturation temperature, i.e.,

$$T_w = T_{ws}. \quad (2-153)$$

2.2.2.3 Transition From Subcooled to Saturated Conditions in the Coolant Region

The transition from the subcooled condition of the coolant, as represented by Equation (2-149), to the saturated condition represented by Equation (2-152) was accomplished by the use of logical control variables.

2.2.2.3.1 Logical Control Variables and Branching Within the Model

As discussed earlier in Section 2.1.1.2, control of computation flow within a model programmed in the MIMIC simulation language is accomplished by the use of logical control variables.

The model presented here was constructed to simulate conditions in the cask both before and after the coolant reached its saturation temperature, i.e.,

$$T_w < T_{ws}, \quad (2-154)$$

and
$$T_w \geq T_{ws}, \quad (2-155)$$

respectively. The logical control variables representing the conditions defined by Equations (2-154) and (2-155) are TLTTS and TGETS, respectively. TGETS is defined by the function switch expression

$$TGETS = FSW(TW-TWS, FALSE, TRUE, TRUE), \quad (2-156)$$

and TLTTS by the logical complement of TGETS

$$TLTTS = NOT(TGETS), \quad (2-157)$$

where

$$TW = t_w,$$

$$TWS = t_{ws}.$$

When Equation (2-155) is true, TGETS is true and TLTTS is false. Conversely, when Equation (2-154) is true, TGETS is false and TLTTS is true.

Logical control variables are also used to control the mode of operation of integration statements in the MIMIC simulation program. This was also discussed in detail earlier in Section 2.1.1.2. The particular application to the present model will be discussed in the following section.

2.2.2.3.2 Integration of the Energy Balances on the Coolant

There are two energy balances on the coolant, one for subcooled conditions (Equation 2-149) and one for saturated conditions (Equation 2-152). When the expression

$$T_w < T_{ws} \quad (2-154)$$

is true, Equation (2-149) is solved for the time derivative of the coolant temperature, dT_w/dt . When the expression

$$T_w \geq T_{ws} \quad (2-155)$$

is true, Equation (2-152) is solved for the rate of change of the mass of coolant in the cask, dM_w/dt . Figure 2-9 shows how the logical control variables TLTS and TGETS are used to flag Equations (2-149) and (2-152) for execution.

After Equations (2-149) and (2-152) have been solved for dT_w/dt and dM_w/dt , respectively, these results are then integrated to give T_w and M_w . The temperature of the coolant is defined by the equation

$$T_w = T_{wi} + \int_0^{t_B} \frac{dT_w}{dt} dt, \quad (2-158)$$

and the mass of coolant remaining in the cask by

$$M_w = M_{wi} + \int_{t_B}^t \frac{dM_w}{dt} dt, \quad (2-159)$$

where

t_B = the time at which $T_w \geq T_{ws}$, θ ,

T_{wi} = the initial temperature of the coolant, T ,

M_{wi} = the mass of coolant in the cask initially, M .

The MIMIC integration statements equivalent to Equations (2-158) and (2-159) are

$$TW = \text{INT}(DTW, TWI, TLTS, \text{TRUE}) \quad (2-160)$$

and

$$MW = \text{INT}(\text{DMW}, \text{MWI}, \text{TGETS}, \text{TRUE}), \quad (2-161)$$

respectively,

where

$$\text{DTW} = dT_w/dt,$$

$$\text{TWI} = T_{wi}$$

$$\text{DMW} = dM_w/dt,$$

$$\text{MWI} = M_{wi}.$$

The logical control variables TLTTTS and TGETS are included in the above integration statements to control the mode of operation of the respective integrators. [Mode-controlled integration is discussed in detail in Section 2.1.1.2, in connection with the general integration statement defined by Equation (2-126), and in Reference (3).]

When TLTTTS is true ($T_w < T_{ws}$), the integrator represented by Equation (2-160) is in the OPERATE mode. This means that the integrator is updated by the MIMIC integration routine and the result of the integration is equivalent to that defined by Equation (2-158). Also, when TLTTTS is true, TGETS is false and the integrator represented by Equation (2-161) is in the HOLD mode. This means that the input to the integrator (dM_w/dt) is removed and M_w is equal to M_{wi} .

When TGETS is true (when $T_w \geq T_{ws}$), TLTTTS is false, and the integrator of Equation (2-160) is now in the HOLD mode. This means that the input to the integrator (dT_w/dt) is removed and T_w is held equal to the last value it had reached, i.e., T_{ws} . Also, when TGETS is true, the integrator represented by Equation (2-161) is now in the OPERATE mode, which means that the integrator is updated and the result of the integration is equivalent to that defined by Equation (2-159).

2.2.2.4 Determination of Temperatures From Energy Balances on the Regions

The energy balances on all the other regions of the cask model are valid throughout the transient, regardless of the state of the coolant. These energy balances have been presented as Equations (2-146), (2-147), (2-148) and (2-150) of Section 2.2.2.1.

Equations (2-146), (2-147) and (2-148) yield the time derivatives of the temperatures of the fuel, basket and cask wall regions, respectively. The temperatures of these regions are obtained by the following integrations:

$$T_F = T_{Fi} + \int_0^t \frac{dT_F}{dt} dt, \quad (2-162)$$

$$T_B = T_{Bi} + \int_0^t \frac{dT_B}{dt} dt, \text{ and} \quad (2-163)$$

$$T_C = T_{Ci} + \int_0^t \frac{dT_C}{dt} dt, \quad (2-164)$$

where T_{Fi} , T_{Bi} and T_{Ci} are the initial temperatures of the regions. The equivalent MIMIC integration statements are:

$$TF = \text{INT}(DTF,TFI), \quad (2-165)$$

$$TB = \text{INT}(DTB,TBI), \quad (2-166)$$

$$TC = \text{INT}(DTC,TCI), \quad (2-167)$$

where

$$DTF = dT_F/dt,$$

$$TFI = T_{Fi},$$

$$DTB = dT_B/dt,$$

$$TBI = T_{Bi},$$

$$DTC = dT_C/dt,$$

$$TCI = T_{Ci}.$$

Note that the integration statements (2-165), (2-166) and (2-167) do not have the third and fourth arguments to control the mode of integration. When the third and fourth arguments of a MIMIC integration statement are missing, the program assumes they are true and the integrator is automatically placed in the OPERATE mode.

The temperature of the cask surface (the outer shell of the water jacket and the fins) may be obtained directly from Equation (2-151).

2.2.2.5 Coolant Loss From the Cask

The rate of loss of the coolant from the cask by vaporization is the time derivative - dM_w/dt . The time to empty the cask is the time required for M_w , as determined from Equation (2-161), to decrease from M_{wi} to 0.

The mass velocity of the coolant vapor leaving the cask through the breach is

$$G_{GAP} = \frac{CF}{A_{GAP}} \left| \frac{dM_w}{dt} \right| \quad (2-168)$$

where

$$A_{GAP} = \text{the area of the breach, in}^2,$$

$$CF = \text{a conversion factor} = 144 \text{ in}^2/\text{ft}^2.$$

3. CASK SIMULATION MODELS FOR LOSS-OF-COOLANT TRANSIENT

Models were developed to simulate the behavior of the IF-300 and AMCO casks following an accident in which the solar shields were lost, along with the water in the outer jackets or neutron shields, and after the casks have lost their primary coolant (cask behavior prior to loss of the primary coolant was simulated using the so-called "coolant loss rate" models discussed in Section 2). The models discussed in this section are referred to as "loss-of-coolant" models.

These loss-of-coolant models are basically heat transfer models, but in addition to the equations describing the heat transfer in the casks they include equations that describe the consequences of loss of the primary coolant. The loss of primary coolant causes overheating of the fuel, which results in expansion of free fission gases in the fuel pins and eventual failure of some fuel pin clads. Failure of the fuel pin clads releases free fission gases and some solid fission products (cesium compounds) to the cask containment, from which they may escape if the containment is breached.

It was stated in the introduction to this Appendix that, at the time the study of spent fuel shipping cask behavior was begun, it was decided to start with the most pessimistic case to determine at the outset the most conservative estimate of fission product release. The most pessimistic case visualized was an accident in which a cask loses its solar shield, the water in its outer jacket, and its primary coolant at the instant the accident occurs. The cask was also assumed to be subjected to a fire at 1475°F for half an hour following the accident. Consequently, the first simulation models constructed were the loss-of-coolant models. At this time, to insure that nothing was overlooked, potential mechanisms governing the possible release of the remaining fission gases bound up in the fuel were included in the model. These potential mechanisms are:

1. oxidation of the UO_2 to U_3O_8 , a loose granular material, from which the bound up fission gases could escape, and

2. diffusion of the bound up fission gases from the fuel if the temperatures were high enough.

As the study progressed, however, it appeared that the probabilities of these mechanisms occurring may be quite small. The diffusional process requires extremely high temperatures to produce a significant release rate. Also, it seems probable that the cask will always be at a pressure higher than the surroundings, so the possibility of air entering the cask to cause oxidation of the fuel seems remote. The equations describing these mechanisms are derived and discussed in this section of the Appendix since they are still part of the present models.

A system of equations was developed that defines the rate of flow of fission gases from the casks through a breach in the containment. This system of equations was developed too late to be included in the present loss-of-coolant models, but the equations will be derived and discussed here, since they will be included in the models during later development phases.

The electrical analogs of the loss-of-coolant models are larger and more complex than those of the coolant loss rate models of Section 2. Consequently, it was not practical to present heat balances for each node as was done for the coolant loss rate models. However, the heat balances are of the same form as those presented in Sections 2.1 and 2.2.

All cask simulation models, except the loss-of-coolant models and the steady-state models, were developed for programming on the MIMIC simulation code.⁽³⁾ The steady-state pre-accident models and the loss-of-coolant models were programmed on the TAP simulation code.⁽⁴⁾ The language and procedures for programming MIMIC closely resemble FORTRAN programming, therefore, MIMIC listings are presented for some of the models, along with a calculation flow diagram or algorithm. The language and procedures for programming a model on TAP, however, are vastly different and unique; consequently, listings of the loss-of-coolant models are not presented, since they would be of little help to one not familiar with the code. However, general algorithms of portions of the models are presented.

A model simulating the transient behavior of the conceptual LWR cask design following an accident and loss of primary coolant was constructed first, but was sufficiently general to be easily adapted to the IF-300 and AMCO designs. Provision was made for melting of the shield in the model of the lead-shielded conceptual cask, but not in the models of the IF-300 or AMCO casks, because melting of the uranium or steel is not likely.

An idealized model of the IF-300 is shown in Figures 3-1 and 3-2. The primary difference between this model and the actual cask is the representation of the fuel, fuel cans, and baskets as circular regions rather than the array of square fuel assemblies (see Figure 3-2). This simplified model was divided into radial nodes as shown in Figure 3-19, and the network of admittances connecting these nodes is shown in Figure 3-20. An idealized representation of the IF-300 was necessary because the array of square fuel assemblies was not symmetrical (see Figure 3-2).

Unlike the IF-300, the arrangement of the fuel assemblies in the containment vessel of the AMCO cask is symmetrical. This allowed the simulation network to be based on a symmetrical cut of the cask as shown in Figure 3-21. In this model, the fuel assembly, the fuel assembly can, and the basket are represented as concentric cylinders divided into radial nodes as shown in Figures 3-3 and 3-21. The baskets surrounding the fuel assemblies are designed with slotted holes for free passage of the liquid coolant under normal conditions. When the primary coolant is lost, these slots allow heat to be transferred by radiation from the fuel can to the expansion chamber wall and to the canister wall. Heat is also transferred by radiation from the outside surface of this basket to the expansion chamber and canister walls.

The loss-of-coolant models were constructed as hybrid-type computer simulations as diagrammed in Figure 3-4. The models consist of three interacting simulation networks (heat transfer, oxidation, and fission

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FIGURE 3-1. Idealized Model of the IF-300 Spent Fuel Shipping Cask

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FIGURE 3-2. Idealized Representation of Fuel Assemblies in the Containment Vessel of the IF-300

HEDL 7507-30.14

FIGURE 3-3. Idealized Representation of a Fuel Assembly in the AMCO Spent Fuel Shipping Cask

HEDL 7507-30.1

FIGURE 3-4. Hybrid-Type Computer Simulation of Spent Fuel Shipping Cask

gas diffusion) and a processor for peripheral computations and logic control. The processor controls the network interactions, melting,* thermal radiation, temperature and time varying inputs, various switching circuits and programming of events. This hybrid-type simulation is accomplished using the TAP (Thermal Analyzer Program) Code.⁽⁴⁾

As discussed earlier, in Section 2.2.2, when the solar shield is lost, the cask is exposed to solar heating. A diurnal variation of the solar heat input was used in both of the loss-of-coolant models discussed here, and in the coolant loss rate model presented in Section 2.2.2. It was assumed that the accident occurs at 6:00 a.m. and that the solar heat falls on the casks at a constant rate until 6:00 p.m. when it drops to zero. This variation of solar heating was programmed into the models as a pulsed function of time where this "on-off" characteristic was repeated as long as required. The solar heat reaching the casks was assumed to be one-third of that which would fall on a flat surface. This was an assumed correction factor to allow for the non-flat, 360° cylindrical surface of a cask. It is impossible for the entire surface of a cask to face the sun.

The cask designs simulated do not have the baskets attached to the inner wall of the containment vessel. If it had been assumed that they had been attached to the containment vessel wall, this would have provided a good path for heat transfer when evaluating conditions following the loss of primary coolant. When bonded to the vessel wall, the baskets act as fins that pick up the heat from the fuel assemblies and transfer it by conduction to the vessel wall. ORNL has assumed this to be the case in some of their earlier studies.⁽¹⁸⁾ When the baskets are not attached to the containment vessel wall, the result is higher fuel temperatures and a shorter time to clad failure and fission product release.

A collection of fuel pins such as in the fuel assemblies have a "lumped" characteristic. It was necessary to devise a method to "distribute"

*This applies only to the lead-shielded conceptual cask.

the "lumped" fuel to give homogeneous regions that could then be "re-lumped" to fit the nodal representation of the networks. This was done by using the concepts of volumetric heat dissipation and an apparent thermal conductivity for materials with voids for heat transfer in the fuel regions, and the concept of volumetric mass dissipation for diffusion of fission gases in the fuel. Representation of the oxidation of the fuel did not require such specialized treatment. The equations defining the heat transfer in the fuel regions, the diffusion of fission gases in the fuel regions, and the oxidation of the fuel, and their electrical analog representations, are presented and discussed in the following sections.

3.1 Heat Transfer in the Fuel

3.1.1 Initial Conditions

The initial conditions used for the transient loss-of-coolant models are the temperature distributions obtained from either the steady-state pre-accident models or the coolant loss rate models at the time the casks have lost all of their primary coolant. This is illustrated in Figure A-1, which shows the flow of information within the system of simulation models developed. The initial temperatures used in the loss-of-coolant model of the IF-300 are the temperatures obtained from its coolant loss rate models. The initial temperatures used in the loss-of-coolant model of the AMCO cask are either the final temperatures obtained from its coolant loss rate model for the breach up position, or from its steady-state pre-accident model if the cask is in the breach down position.

3.1.2 Volumetric Heat Dissipation

Due to the complexity posed by the "lumped" nature of the fuel pin bundles, the concept of volumetric heat dissipation, along with that of an apparent thermal conductivity, was used to simplify the simulation of the heat transfer in these bundles or assemblies. These concepts were used to "distribute" the "lumped" fuel to convert the fuel assemblies into

homogeneous regions which could then be "re-lumped" into nodes for the heat transfer network. The concept of volumetric heat dissipation was also used in the development of the steady-state pre-accident models of Section 1 and the coolant loss rate models of Sections 2.1 and 2.2.

The concept of volumetric heat dissipation and the derivation of a volumetric heat dissipation coefficient have been developed in detail in Section 1.2. The volumetric heat dissipation coefficient is based on the coefficient for heat transfer by natural convection from the fuel pins to the coolant. The natural convection coefficient in Section 1.2 is defined by Equation (1-16), which is McAdam's equation for liquids heated outside single horizontal tubes.⁽¹⁶⁾

Results from the coolant loss rate models indicate that some residual coolant vapor will remain in the casks after the liquid coolant is gone. This is clearly evident in the case of the IF-300 where the results show that, when the pressure in the cask drops to atmospheric pressure, about 2.0 pounds of steam are left in the cask. This coolant vapor will circulate in the fuel assemblies and in the cask cavity by natural convection, transferring heat from the fuel pins to the inside surface of the cask cavity in the same way the liquid coolant did earlier.

The coefficient for heat transfer from the fuel pins to the coolant vapor is also defined by Equation (1-16), which Stoevers⁽¹⁶⁾ states is valid for gases heated by natural convection outside single horizontal tubes. Stoevers has evaluated Equation (1-16) for various gases and has presented the results as a base heat transfer coefficient, h_o , which is a function of the temperature difference between the tube surface and the gas [see Equation (1-17)].

The base coefficient is multiplied by temperature, pressure and tube diameter correction factors to give the heat transfer coefficient for any combination of film temperature, cavity pressure and tube size:

$$h = h_o F_t F_p F_d \quad (3-2)$$

where

F_t = the temperature correction factor

F_p = the pressure correction factor

F_d = the tube diameter correction factor.

This was the same procedure followed in Section 2.1.1.3.1. The factors F_t and F_d are defined by Equations (1-19), (1-20), and (1-21) in Section 1.2, and the factor F_p by Equation (2-81) in Section 2.1.1.3.1. Values of these factors are tabulated in Reference 16.

Equivalent forms of Equations (3-2), (1-19), (1-20), (1-21), and (2-81) are programmed into the model to provide the correct heat transfer coefficient during computation of the transient temperatures in the cask.

Dowtherm-A vapor was not among the gases included on Stoevers' charts, therefore, it was assumed that this vapor could be represented by steam.

It should be mentioned here that, in both the steady-state pre-accident models and the loss-of-coolant models, the coefficient for the transfer of heat by natural convection from the coolant in the cask cavity to the inner surface of the cask cavity was determined using a procedure similar to that outlined here and in Sections 1.2 and 2.1.1.3.1. However, a different heat transfer coefficient equation was used. It was assumed that heat transfer to the inner surface of the cask cavity, and in the outer water jacket, would be the same as that to vertical plates.

The Colburn and Hougen equation was used to determine the heat transfer for both liquids and gases heated by natural convection on vertical plates⁽¹⁶⁾

$$h = 0.128 \left(\frac{k^3 \rho^2 C_p g (\Delta t)}{\mu} \right)^{1/3} . \quad (3-3)$$

See Equation (1-16) in Section 1.2 for the definitions of the terms used in the above equation.

3.1.3 Heat Conduction and Apparent Thermal Conductivity

When the cask loses its coolant due to the accident, the Maxwell equation is no longer appropriate for determining the apparent thermal conductivity. For this case, a fuel assembly was represented by a fuel pin at the center of the assembly surrounded by a series of concentric "cans" made of fuel material, as shown in Figure 3-5. The cans are separated by spaces filled with residual steam. Heat is assumed to be transferred from the center pin to the nearest can, and from can to can, by radiation and conduction, and by conduction across the can walls. Heat transfer by radiation through the spaces between the fuel pins was not allowed. The apparent thermal conductivity for this configuration was determined using the Eucken-Nusselt equation for a body composed of a system of alternate parallel solid plates and steam gaps,⁽¹⁶⁾

$$k_a = \frac{L_{13}}{\frac{L_{12}}{k_s} + \frac{L_{23}}{k_{g,r}}} \quad (3-4)$$

where

L_{12} = the thickness of the plate or can wall, L

L_{23} = the thickness of the gap separating the cans, L

L_{13} = $L_{12} + L_{23}$, L

$k_{g,r}$ = the thermal conductivity of the gap, including the effect of radiation, H/θLT.

The thermal conductivity, $k_{g,r}$, is obtained by combining the heat transferred across the gap by conduction with that transferred by radiation. The heat transferred across the gap is

$$q_{23} = q_c + q_r = \frac{k_{g,r}}{L_{23}} A (T_2 - T_3), \quad (3-5)$$

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FIGURE 3-5. Representation of PWR Fuel Assembly as a Collection of Concentric Cans

where the conduction component is

$$q_c = k_g \frac{A}{L_{23}} (T_2 - T_3) \quad (3-6)$$

and the radiation component is

$$q_r = A F_{23} \sigma (T_2^4 - T_3^4) \quad (3-7)$$

where

F_{23} = the combined emissivity and shape factor for
radiant energy transfer between surfaces 2
and 3

σ = the Stefan-Boltzmann constant, $H/\theta LT^4$.

If the radiation component is written in terms of an equivalent thermal conductivity for radiation, then Equation (3-7) becomes

$$q_r = k_r \frac{A}{L_{23}} (T_2 - T_3) \quad (3-8)$$

where

k_r = the equivalent thermal conductivity for radiation,
 $H/\theta LT$.

Since Equations (3-7) and (3-8) are equivalent, they may be combined to give

$$k_r \frac{A}{L_{23}} (T_2 - T_3) = A F_{23} \sigma (T_2^4 - T_3^4), \quad (3-9)$$

or

$$k_r = \frac{F_{23} \sigma (T_2^4 - T_3^4) L_{23}}{T_2 - T_3} . \quad (3-10)$$

If T_2 is nearly equal to T_3 , then differentials may be used in Equation (3-10) instead of the differences,

$$k_r = F_{23} \sigma \frac{dT^4}{dT} L_{23} . \quad (3-11)$$

Now

$$\frac{d}{dT} (T^4) = 4T^3, \quad (3-12)$$

therefore Equation (3-11) becomes

$$k_r = 4F_{23} \sigma T^3 L_{23} . \quad (3-13)$$

Substitution of Equations (3-6) and (3-8) into (3-5) yields

$$k_{g,r} \frac{A}{L_{23}} (T_2 - T_3) = k_g \frac{A}{L_{23}} (T_2 - T_3) + \frac{k_r A}{L_{23}} (T_2 - T_3)$$

or

$$k_{g,r} = k_g + k_r . \quad (3-14)$$

Substituting from Equation (3-13) gives

$$k_{g,r} = k_g + 4F_{23} \sigma T^3 L_{23} . \quad (3-15)$$

The apparent thermal conductivity is then obtained by substituting the expression for $k_{g,r}$ in Equation (3-4),

$$k_a = \frac{L_{13}}{\frac{L_{12}}{k_s} + \frac{L_{23}}{k_g + \frac{4\epsilon_{23} \sigma T^3 L_{23}}{L_{23}}}} \quad (3-16)$$

The heat transferred between fuel nodes in the heat transfer network is:

$$q = \frac{k_a A}{L} (T_{m+1} - T_m) = Y_K (T_{m+1} - T_m) \quad (3-17)$$

where

q = the heat transferred, H/θ ,

A = the heat transfer area, L^2

L = the path length, L

T_m = temperature of node m , T ,

Y_K = the heat conduction admittance, $H/\theta T$.

= $k_a A/L$.

3.2 Fission Product Release Mechanisms

Several possible mechanisms for the release of fission products from the spent fuel were postulated during the initial phases of model construction. Other possible mechanisms were suggested later as more information became available and the results of cask behavior were revealed by analyses using the simulation models. Since most of the fission products that could be released from the fuel assemblies in the casks are fission gases and volatile solids or solid fission products (cesium compounds), the mechanisms governing their release were included early in the development of the loss-of-coolant models.

During reactor operation, fission gases are generated. Some of these gases migrate to the fuel pin voids, i.e., the space between the clad and the fuel, between fuel pellets, and in the plenum or expansion chamber at the end of a pin. These are referred to in this report as "free" gases.

An evaluation of the fission product release from the IF-300 was made assuming that the seven fuel assemblies in the cask were the Design Basis PWR 1 fuel assemblies of Table III-1 in Reference 1. Characteristics of this fuel are presented in Tables 1 and 2. The calculated fission product inventory and activity for this spent fuel after 90 days cooling time were derived from data presented in References 1 and 14. The fission products considered and the number of grams and curies of each in the inventory are given in Table 3-1. According to Reference 1, only about 33% of the fission gases in this inventory (35% of the Kr-85 and I-129, and 3% of the Xe and I-131) is expected to migrate to the fuel pin voids during reactor operation and be available for release if the clads burst. The calculated amounts of radioactivity in the fission products generated in the Design Basis PWR 1 fuel and the amounts that have migrated to the fuel pin voids are presented in Table 3-2. The radioactivity of the fission products in the spent fuel in the IF-300 and the estimated amounts released are presented in Table 3-3.

The AMCO cask carries nine fuel assemblies of the type shown in Figure 6. It was assumed that these fuel assemblies were average assemblies, i.e., each had been operating in the reactor at an average power of 5.2 MW. The

TABLE 3-1

Comparison of Fission Product Inventories Calculated to Be Present in the IF-300 Design Basis PWR 1 Spent Fuel and in Spent Diablo Canyon Reference PWR Fuel.

(Compiled from References 1 and 14)

Fission Product Inventories				
Cooling Time = 90 Days				
Isotope	IF-300 Design Basis PWR 1 Spent Fuel ⁽¹⁾		Spent Diablo Canyon Reference PWR Fuel ⁽¹⁴⁾	
	Total Generated* (C _i /MTU)	Total Generated* (Grams/MTU)	Total Generated** (C _i /MTU)	Total Generated** (Grams/MTU)
Kr	10500.	377.	11300.	374.
Xe	169.	5836.	117.	5420.
I	535.	249.	381.	271.
Cs	~353000.***	~2910.***	333000.	2740.
TOTALS	364204.	9372.	344798.	8805.

$$* E = 35 \frac{\text{GWD}}{\text{MTU}}$$

$$P_o = 40 \frac{\text{Kw}}{\text{KgU}}$$

$$** E = 33 \frac{\text{GWD}}{\text{MTU}}$$

$$P_o = 30 \frac{\text{Kw}}{\text{KgU}}$$

*** The amounts shown here are reasonably close despite the differences in conditions. Tables IX-1 through IX-3 in Reference 1 indicate that changes in inventory due to specific power are small while the changes due to exposure are large, therefore, approximate concentrations for cesium were obtained by multiplying the values for the Diablo Canyon fuel by the ratio of the exposures.

TABLE 3-2

Calculated Amounts of Radioactivity in Fission Products Generated in Design Basis PWR 1 Fuel and the Amounts That Have Migrated to the Fuel Pin Voids

(Compiled from data presented in References 1 and 14)

Fission Product Inventory				
Cooling Time = 90 Days				
Isotope	Total Generated in the Fuel (C _i /MTU)	Total in the Fuel Pin Voids (C _i /MTU)	Total Generated Present in 7 Fuel Assemblies (Curies)	Total in the Pin Voids in 7 Fuel Assemblies (Curies)
Kr-85	10500.	3675.*	33339.60	11668.86
XE-131m	150.	4.5**	476.21	23.81
XE-133	19.	0.6**	60.2	3.01
I-129	0.03	0.01**	0.098	0.0049
I-131	535.	16.1**	1698.69	84.934
Cs	353000.	3530.***	1120838.24	11208.382
Total Fission Gases	11204.03	3696.21	35574.798	11780.618****
Total Cesium	353000.	3530.	1120838.24	11208.382****
Total Fission Products	364204.03	7226.21	1156413.04	22989.0

* Based on 35% migration to pin voids.

** Based on 5% migration to pin voids.

*** Based on 1% migration to pin voids.

**** These values are about 1% less than those used in the model due to slight conversion errors.

TABLE 3-3

Radioactivity of the Fission Products in the Spent Fuel in the IF-300 and Estimated Amounts Released.

Fuel Node in Loss-of- Coolant Model	Initially in the Fuel			Released from the Fuel		
	Fission Gases (Curies)		Cesium (Curies)	Fission Gases (Curies)		Cesium (Curies)
	Kr	Xe + I		Kr	Xe + I	
1	792.3	53.2		277.3	1.596	
2	2376.2	159.5		831.7	4.785	
3	1659.	111.3		580.7	3.34	
7	6200.	416.1		2170.	12.48	
8	8712.6	584.7		3049.	17.54	
9	10296.6	691.		3604.	20.73	
10	3774.2	253.3		1321.	7.6	
Totals	33810.9	2269.1	11208.382	11833.7	68.07	112.08
TOTALS	36080.		11208.382	11901.77*		112.08*

* These values are slightly less than those obtained from the model due to small conversion errors.

calculated fission product inventory and activity for this spent fuel after 120 days cooling time were derived from results presented in Reference 11 for FFTF fuel assemblies that had been operating at 7.0 MW each. The fission gases considered and the number of gram-atoms of each in the FFTF fuel are presented in Table 3-4. The calculated radioactivities of these fission gases are presented in Tables 3-5 and 3-6. The fraction of this inventory of fission gases that is expected to migrate to the fuel pin voids during operation and be available for release, if the clads burst, was calculated using the following equation⁽¹⁹⁾

$$f = 1 - \frac{\left[\frac{1 - \exp(-6.84 \times 10^{-5} B)}{6.84 \times 10^{-5} B} \right]}{\left[0.421 \exp(0.05Q) \right]} \quad (3-18)$$

where

- f = the fractional release
- Q = the local linear heat rate, kw/ft
- B = the local burnup, MWD/MT.

It was determined that the local linear heat rate was about 8 kw/ft. The local burnup was about 50,000 MWD/MT. Using these input values, a fractional release of 0.56 was calculated using Equation (3-18).

The remaining fission gases produced are bound up in the interstices of the fuel material and are referred to as "bound up" gases in this report.

The equations describing the various fission product release mechanisms and an explanation of how they were incorporated into the loss-of-coolant models are presented in the following sections. The mechanisms to be discussed are:

1. Fuel pin clad failure caused by expansion of the free gases, resulting in their release,
2. Diffusion of the bound up fission gases from the fuel following clad failure, and

TABLE 3-4

Total Amounts of Significant Gaseous Fission Product Elements Calculated to be Present in Spent FTR (FFTF) Fuel - 100 Days Decay Time[†].

(Reference 11)

Element	Gram - Atoms*	Gram - Atoms Per Pin**
H (Tritium)	Negligible	-
Kr	10.30	0.00650
I	7.64	0.000482
Xe	108.50	0.006849
Br	Negligible	-
TOTALS	126.44	0.007981

* No. of metric tons charged = 2.52

** 73 drivers with 217 pins each = 15,841 pins

† Good for decay times of 100 days and 120 days

Conditions:

1. Power = $159 \frac{\text{MW}}{\text{MT}}$ (400 MW in FTR)

2. Burnup = $50000 \frac{\text{MWD}}{\text{MT}}$

3. Flux = $7 \times 10^{15} \text{ n/cm}^2\text{-sec}$

TABLE 3-5

Calculated Radioactivity (Total) of Gaseous
Fission Product Elements Present in Spent
FFTF Reference Core Fuel
(120 Days Decay Time)

(Reference 11)

Element	Curies, per Metric Ton Charged*	Curies	Ave. Curies per Pin**	Percent
Kr ₈₅	9,115.	22,969.800	1.39278	97.69
Xe _{131m}	69.60	175.392	0.01063	0.75
Xe ₁₃₃	1.40	3.528	0.00021	0.02
I ₁₃₁	144.	362.880	0.02200	1.54
I ₁₂₉	0.51	1.285	0.00008	0.01
TOTALS	9,330.51	23,512.885	1.42570	100.01

* No. of metric tons charged in FTR = 2.52.

** No. of fuel pins in the core = 16,492 (includes equivalent drivers
in test elements).

Conditions:

1. Power = $159 \frac{\text{MW}}{\text{MT}}$
2. Burnup = $48,000 \frac{\text{MWD}}{\text{MT}}$
3. Flux = $7 \times 10^{15} \text{ n/cm}^2\text{-sec}$

TABLE 3-6

Radioactivity in the Fission Gases in the
AMCO Spent Fuel Shipping Cask
(120 Days Decay Time)*

Node in Loss-of-Coolant Model	Free Gases (Curies)	Bound up Gases (Curies)	Total Gases (Curies)
1	74	58	132
2	221	174	395
3	369	290	659
4	520	408	928
5	354	278	632
TOTALS	1538	1208	2746

* Based on nine average fuel elements in the cask, each of which had been operating at 5.2 MW.

3. Release of bound up fission gases following disintegration of the fuel due to oxidation. If failure of the pin clads exposes the fuel to air in the containment vessel, the UO_2 will oxidize to U_3O_8 , a loose granular material, from which the bound up gases are released.

3.2.1 Fuel Pin Internal Pressures and Clad Stresses

The pressure buildup of the fission gases in the pins as a function of time following loss of the primary coolant is presented in Figures 3-6 through 3-9 for the IF-300, and in Figure 3-10 for the AMCO cask. The pressure in the pin voids is plotted for each fuel node of the cask simulation models shown in Figures 3-19, 3-20, and 3-21. The pressure which gives a hoop stress exceeding the creep rupture strength of the pin cladding at the fuel node temperature is also shown in Figures 3-6 through 3-9 as the burst pressure.

The void region in the fuel pin consists of the plenum space, the gap between the fuel and the clad, and the spaces between fuel pellets. The plenum space for a reference pressurized water reactor (PWR) fuel pin is illustrated in Figure 4, and the pertinent design dimensions are given in Table 2.^(1,8) The length of the plenum space in the FFTF driver fuel pin carried in the AMCO cask is presented in Table 4.

The circumferential or hoop stresses in the cladding of the pins in the fuel nodes are presented as functions of time after impact and fire in Figures 3-11 through 3-14 for the IF-300, and in Figure 3-15 for the AMCO cask. These figures not only show the hoop stresses as functions of time, but also present creep rupture strength curves for the pin clads in each node. The node temperatures are implicit in the results.

The strength of the fuel pin clad material is an important factor in determining the time when the clads will fail. The pin clads will fail when the hoop stresses exceed the strength of the clad material. At the present stage of model development, the strength of the clad material is assumed to follow a creep rupture strength vs. temperature relationship. This is only temporary until the model can be modified to calculate cladding failure based on the time-temperature dependent creep-rupture technique of

FIGURE 3-6. Pressures in the Fuel Pins in the IF-300 (Zircaloy-4, 10 Hour Creep Rupture)

FIGURE 3-7. Pressures in the Fuel Pins in the IF-300 (Zircaloy-4, 10 Hour Creep Rupture)

FIGURE 3-8. Pressures in the Fuel Pins in the IF-300 (Zircaloy-4, 10 Hour Creep Rupture)

FIGURE 3-9. Pressures in the Fuel Pins in the IF-300 (Zircaloy-4, 10 Hour Creep Rupture)

FIGURE 3-10. Pressures in the Fuel Pins in the AMCO Cask for Breach Areas of 0.025 and 0.25 Sq. Inches (for Cask in Breach Down Position)

FIGURE 3-11. Fuel Pin Clad Stresses in the IF-300 (Zircaloy-4, 10 Hour Creep Rupture)

FIGURE 3-12. Fuel Pin Clad Stresses in the IF-300 (Zircaloy-4, 10 Hour Creep Rupture)

FIGURE 3-13. Fuel Pin Clad Stresses in the IF-300 (Zircaloy-4, 10 Hour Creep Rupture)

FIGURE 3-14. Fuel Pin Clad Stresses in the IF-300 (Zircaloy-4, 10 Hour Creep Rupture)

FIGURE 3-15. Fuel Pin Clad Stresses in the AMCO Cask for Breach Areas of 0.025 and 0.25 Sq. Inches (for Cask in Breach Down Position)

Reference 20. The PWR fuel pin clads are Zircaloy-4. For this alloy, a 10 hour creep-rupture strength vs. temperature relationship from the Cask Designer's Guide (Reference 7, page 154) was used. The FFTF driver fuel pin clads are Type 316 stainless steel. A 100 hour creep-rupture vs. temperature curve from Reference 21 was used for these clads. These curves, or their equivalent, were programmed into the TAP loss-of-coolant models as controls. The calculated hoop stresses in the clads are compared to the clad strengths by a control function in the central processor, and when they exceed the strength, it represents failure of the clad. When this happens, a "switch" is activated that controls the release of the free fission gases in the pin void spaces, the onset of oxidation of the fuel leading to the release of bound up fission gases, and the diffusion of bound up gases through the fuel.

The internal pressures in the pins and the stresses in the clads are calculated as functions of temperature by the central processor as follows:

For thin-walled cylinders, the hoop stress, S , in the cylinder wall is related to the internal pressure, P , in the cylinder by the equation

$$\frac{\Delta P}{S} = \frac{2(R_o - 1)}{(R_o + 1)} \quad \text{for } R_o < 1.20 \quad (3-19)$$

where

$$\begin{aligned} R_o &= \text{the ratio of the outside diameter of the cylinder or} \\ &\quad \text{clad to the inside diameter} \\ &= \frac{d_o}{d_i} \end{aligned} \quad (3-20)$$

$$\begin{aligned} \Delta P &= \text{the pressure differential across the clad} \\ &\quad \text{wall, } \frac{F}{L^2} \\ &= P - P_{\text{CAVITY}} \end{aligned} \quad (3-21)$$

P_{CAVITY} = the pressure in the cask cavity, $\frac{F}{L^2}$.

The outside diameters of the clads and their thicknesses, t , are specified in Table 2 and Table 4, therefore,

$$d_i = d_o - 2t . \quad (3-22)$$

As an example, for the PWR fuel pin

$$R_o = \frac{d_o}{d_o - 2t} = \frac{0.460}{0.460 - 0.04} = 1.095 < 1.20 \quad (3-23)$$

and
$$\frac{\Delta P}{S} = \frac{2 (R_o - 1)}{(R_o + 1)} = 0.0907 \quad (3-24)$$

or
$$S = 11.03 \Delta P . \quad (3-25)$$

The stresses in the fuel pin clads in the AMCO cask were not calculated directly by the simulation model. Instead, experimental data on burst pressures as a function of temperature for Type 316 stainless steel clads (Reference 21, Table 16) were programmed into the model for monitoring clad failure. The clad stresses were calculated later from pressures obtained from the model.

For the IF-300, the internal pressure in a pin is calculated from the equation⁽⁷⁾

$$P = (P'f + P_o) \frac{T}{T_o} \quad (3-26)$$

where:

P = the total gas pressure, F/L^2

P' = the pressure at T_o , resulting from 100% release of fission gases from the fuel pellets, F/L^2

f = the fraction of gases released from the pellets to the pin plenum

P_o = the initial fill pressure at T_o , F/L^2 (taken to be 55 psia at 100°F)⁽¹⁾

$\frac{T}{T_o}$ = the ratio of the absolute temperature of the node representing the fuel region containing the pin to the base absolute temperature (temperatures in °R).

The product $P'f$ represents the pressure of the gases actually released from the fuel pellets.

The pressure P' is calculated from the gas law

$$P' = \frac{NRT}{V'} \quad (3-27)$$

expressed as

$$P' = \frac{1.45 E R T_o}{V'} \quad (3-28)$$

where 1.45 = the total gas generation, Gm atoms/GWD

E = the exposure, GWD/MTU

R = the gas constant

= 40.84 (psia-in³)/(Gm-mole°R)

V' = the specific gas collection volume, in³/MTU.

Fuel pin gas collection volumes for several pressurized water reactors are listed in Table IX-6 of Reference 1. An average of these is $V' = 569$ in³/MTU. The worst case PWR design basis fuel was assumed for this study. The fission product inventory for this fuel is summarized in Table 3-1, and in Table IX-9 in Reference 1. For this fuel,

$E = 35$ GWD/MTU,

$P_o = 40$ Kw/KgU,

and the cooling time is 90 days following reactor shutdown. Using the above values of E and V' , and Equation (3-28), P' was calculated to be 2040 psia. Using a release fraction of 0.35 for all the fission gases, the pressure of the gases released to the pin voids is

$$\begin{aligned}
 P'f &= (2040)(0.35) \\
 &= 714 \text{ psia.}
 \end{aligned}$$

This gas pressure, along with the initial fill pressure and temperature, was used in Equation (3-26) to obtain the final form of the pressure equation to be used in the model:

$$\begin{aligned}
 P &= (P'f + P_o) \frac{T}{T_o} & (3-26) \\
 &= (714 + 55) \frac{T}{560} \\
 &= 1.373T \\
 &= 1.373(T_f + 460) & (3-29)
 \end{aligned}$$

where T_f = the temperature of the node representing the fuel region containing the pin, °F.

The internal pressures in the fuel pins in the AMCO cask were determined using a different approach. It has been estimated that the end-of-life pressure in these pins is about 750 psia at 1100°F.⁽³³⁾ It was assumed that this pressure could be expressed as

$$P' = \frac{R}{V}(T_f + 460) , \quad (3-30)$$

or
$$750 = \frac{R}{V}(1100 + 460) .$$

The term $\frac{R}{V}$ was obtained by solving Equation (3-30) to give

$$\frac{R}{V} = \frac{750}{1560} = 0.48 .$$

Since the product $P'f$ represents the pressure of the gases actually released to the pin voids, Equation (3-30) may be rewritten as

$$P = P'f \quad (3-31)$$

$$= \frac{Rf}{V}(T_f + 460) \quad (3-32)$$

$$= 0.48f(T_f + 460) , \quad (3-33)$$

where f is the fractional release defined by Equation (3-18). This fractional release was calculated to be 0.56. Therefore, Equation (3-33) reduces to

$$P = 0.27(T_f + 460) . \quad (3-34)$$

Equation (3-33) is part of the AMCO cask model and, during a simulation, the pressures obtained from this equation are compared to burst pressure vs. temperature data. When

$$P \geq P_{\text{Burst}} , \quad (3-35)$$

the pin clads fail, releasing the fission gases in the pin voids.

The stresses in the fuel pin clads in the AMCO cask were calculated later, using Equation (3-19) and the pressures obtained from Equation (3-33) during the simulation.

The failure of a pin clad in the simulation models not only signals the release of free gases from the pin void space, it also controls the release of bound up gases from the fuel by oxidation and diffusion. The activation of these release mechanisms is controlled by algorithms programmed into the central processor of the models. These algorithms for the IF-300 model are shown in Figures 3-16 and 3-27. The algorithms for the AMCO cask model are somewhat different due to the differences in the two approaches discussed above.

In Figure 3-16, the strength, SU_m , of the pin clads in fuel region m is determined as a function of the node temperature T_m . The internal pressure, P_m , is determined from Equation (3-29) in the form shown. Once P_m is determined, the clad hoop stress, S_m , is then calculated. The clad stress

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FIGURE 3-16. Algorithm Controlling Simulation of Release Mechanisms
(Page 1 of 2)

HEDL 7507-30.23

FIGURE 3-16. Algorithm Controlling Simulation of Release Mechanisms
(Page 2 of 2)

is compared to the clad strength and, if $S_m \geq SU_m$, the switching variable D3 is set equal to one. If $S_m < SU_m$, D3 is set equal to zero. Admittances attached to node m in the oxidation and diffusion networks are activated or remain inactive, depending on the value of D3.

Also, in the algorithm of Figure 3-16, the reaction rate constant, K_{pm} , and the diffusion coefficient $DPRIME_m$, are shown as functions of the fuel node temperature. The typical oxidation reaction admittance, Y_C , is determined as a function of the reaction rate constant and the node oxygen concentration, M_m , from the oxidation network. The typical diffusion admittance, Y_D , is determined as a function of the diffusion coefficient, but is independent of the fission gas concentration.

The release of the free fission gases in the pin voids is also controlled by the switching variable D3. The total number of moles, ML_m , of fission gas in a fuel node, both free and bound up, is first multiplied by F_G to convert it to the number of moles of free fission gases in the pin voids. This modified value of ML_m is then multiplied by D3 and read out as a function of time. Finally, ML_m is multiplied by a conversion factor, C/M, which is the number of curies present in a mole of gas, to get the total curies radioactivity, CI_m , released from node m.

3.2.2 Diffusion of Fission Gases from the Fuel

Results using the loss-of-coolant models have shown that the amount of fission gases released from the spent fuel by diffusion is negligible. The spent fuel temperatures never reach a level high enough to produce a diffusion coefficient large enough to allow other than negligible amounts of gas to be released. However, since this release mechanism is included as part of the model, the concepts and equations developed will be presented in the following sections.

3.2.2.1 Volumetric Mass Dissipation

Diffusion of fission gases in a "unit cell" is illustrated in the following sketch, and defined by Equation (3-36).

$$-V \frac{d\bar{N}}{dt} = J \frac{DA}{L} (\bar{N} - \bar{N}_0) \quad (3-36)$$

where

- V = the volume of fuel, L^3
- $\bar{N}$ = the average fission gas concentration in the fuel, M/L^3
- $\bar{N}_0$ = the concentration of fission gas in the voids, M/L^3
- t = time, θ
- D = the coefficient for diffusion of fission gases through the fuel, L^2/θ
- A = the surface area of the fuel pin, L^2
 $= 2\pi a \Delta x$
- L = the diffusion path length, L
 $= a$
- J = the mass of fission gas transferred, M/θ .

The mass transfer from the pin to the voids is

$$J = \frac{2\pi a D}{a} (\bar{N} - \bar{N}_0) \Delta x \quad (3-37)$$

In volumetric terms, the mass transfer may be expressed as

$$J = \pi b^2 D_v (\bar{N} - \bar{N}_0) \Delta x \quad (3-38)$$

where

D_v = the volumetric mass dissipation coefficient, $\frac{1}{\theta}$.

Substituting from Equation (3-37) into Equation (3-38), rearranging, and using Equation (1-11), the volumetric mass dissipation coefficient is defined as

$$D_v = \frac{2D}{a^2} (1-B) . \quad (3-39)$$

Equation (3-38), rewritten on a nodal basis for the diffusion network, is

$$J = Y_D (\bar{N} - \bar{N}_0) \quad (3-40)$$

where

Y_D = the mass dissipation admittance, L^3/θ

$$= D_v S_{\text{node}} \Delta x . \quad (3-41)$$

Substituting from Equation (3-39), Equation (3-41) becomes

$$Y_D = \frac{2D}{a^2} (1-B) S_{\text{node}} \Delta x . \quad (3-42)$$

3.2.2.2 Diffusion Network

It was assumed that the fission gases will not diffuse from pin to pin since the flow path through the voids (coolant space) is the path of least resistance. Assuming only diffusion to the voids, the network for one fuel node is shown in the following sketch.

The capacitance of the fuel node in this basic network is the volume of the fuel. The sink or void gas concentration, $\bar{N}_0$, is assumed to be 0.

3.2.2.3 Coefficient for Diffusion of Fission Gases in the Fuel

An empirical diffusion coefficient was used to calculate the diffusion of fission gases through the fuel. According to Allen,⁽²²⁾ the empirical diffusion coefficient is related to the actual diffusion coefficient by the expression:

$$D' = \frac{D}{a^2} \quad (3-43)$$

where

$$a = \frac{3}{S} \quad (3-44)$$

S = the surface area per unit volume of the bulk fuel, 1/cm,

a = the radius of hypotheticalal spheres which, it is assumed, constitute the UO_2 , cm.

For a basic sphere,

$$S = \frac{4\pi a^2}{\frac{4}{3}\pi a} = \frac{3}{a} \quad (3-45)$$

It was assumed that the diffusion of the fission gases would be similar to the diffusion of xenon alone, and that the coefficient for the diffusion of xenon through UO_2 would be representative of the diffusion coefficient for the fission gases. ORNL-4228 (Reference 23) presents a plot of the log of the diffusion coefficient for xenon as a function of the reciprocal of the absolute temperature. This plot was represented approximately by the equation

$$\text{Log } D' = -1.32 \left(\frac{10^4}{T} \right) - 1.0 \quad (3-46)$$

where

T = the absolute temperature, $^{\circ}\text{K}$,

D' = the empirical diffusion coefficient, $\frac{1}{\text{sec}}$.

The plot in Reference 23 did not extend the temperature range below about 1000°K (1340°F). Therefore, extrapolations were made to lower temperatures, using Equation (3-46). The empirical diffusion coefficient for xenon used in this study, based on extrapolations using the above equation, is shown in Figure 3-17.

Calculated results have shown that the amount of fission gases released by diffusion from the fuel is negligible. The diffusion process is extremely slow, even at the highest temperatures reached during the simulation.

If oxidation of the solid UO_2 to the granular or loose U_3O_8 occurs, the diffusion coefficient might improve drastically at the conversion point in a step-wise manner, rather than remaining a straight line function as indicated in Figure 3-17. The following sketch illustrates how the "improved" diffusion coefficient might appear on a $\text{Log } D'$ versus $\frac{1}{T}$ plot.

FIGURE 3-17. Empirical Diffusion Coefficient for Xenon (Reference 23)

In this study it was assumed that the fission gases would be released instantaneously if the UO₂ is converted to U₃O₈ which, in effect, implies that the diffusion coefficient goes to a very large value in a step manner.

The diffusion coefficient was not corrected for the effect of burnup while the fuel was in the reactor. The data of Daniel, Evans and Shilling⁽²⁴⁾ indicate that the diffusion coefficient could be higher by as much as a factor of 30. Even if this factor were applied in this study, diffusion would still be negligible.

3.2.3 Oxidation of the Fuel

Another mechanism included in the loss-of-coolant models for the release of "bound up" gases and solids from the fuel is oxidation of the UO₂ to U₃O₈. U₃O₈ is a fine granular material from which these bound up gases and solids can more easily be released. However, as the study progressed, results from use of the chain of simulation models seemed to indicate that this mechanism would be less likely to occur than originally thought. The results indicated that the cask would probably always be at a pressure

higher than its surroundings. This would prevent any air from entering the cask.

There are at least two reasons why the pressure in the cask may be higher than the pressure of the surroundings. First, residual coolant vapor may be present in the cask for some time following the loss of primary coolant. The pressure of this residual vapor would increase as it is heated. Second, the fission gases released from the fuel pins are at the burst pressure of the pin clads. Although these pressures will drop to some lower value as the gases expand into the cask containment, they will increase again as the gases are heated by the fuel assemblies.

Oxidation of the fuel by the water vapor in the IF-300 has not yet been evaluated, but it is not expected to be significant.

Fuel oxidation as a release mechanism is part of the loss-of-coolant models, so the concepts and equations that describe this mechanism will be presented in the following sections.

3.2.3.1 Parabolic Rate Law

Fuel, exposed to the atmosphere after clad failure, was assumed to be oxidized according to the parabolic rate law.

$$X = \sqrt{kt} \quad (3-47)$$

where

X = the thickness of a second-phase oxide product, L

k = the reaction constant, $\frac{L^2}{\theta}$

t = the time, θ .

This equation was converted to a mass-based rate law for the simulation of fuel oxidation. This mass-based law, as developed later in this section, is

$$M^2 = K_p t \quad (3-48)$$

where

M = the mass of oxygen consumed, or the mass gain of the oxide product, M/L^2

K_p = the mass-based rate constant, $M^2/L^4\theta$
= $\rho^2 k$

ρ = the second phase oxide product density, $\frac{M}{L^3}$.

The time derivative of Equation (3-48),

$$2M \frac{dM}{dt} = K_p, \quad (3-49)$$

was used as the basis for the oxidation network. In the simulation of oxidation using Equation (3-49), K_p is a function of temperature (see Table 3-7 and Figure 3-18), and the fuel pellets are assumed to be spheres.

The heat of oxidation was not considered in the simulation; however, this could be included in the model later. This would be one of the interactions between the oxidation network and the heat transfer network.

Oxidation of the fuel might be impeded by lack of oxygen, since the fire would probably consume most of the oxygen in the immediate vicinity. In this study, it was assumed that the fuel would be exposed to a normal atmosphere in which the oxygen is not depleted by combustion of the petroleum, and therefore oxidation of the fuel would be reaction rate-controlled. An oxygen supply-limited reaction model may be used later rather than the rate-controlled model if it is possible to estimate the amount of oxygen (air) reaching the exposed fuel.

3.2.3.2 Oxidation Network

The oxidation of the fuel is a function of the temperature of a fuel node only, not of the "lumped" or "distributed" representation of the node. It is based upon the behavior of a representative pin in the node, not on the node as a set of pins.

Oxidation of the fuel was simulated by converting Equation (3-49) to a mass conservation equation

$$\frac{dM}{dt} = Y_o (M_o - M) \quad (3-50)$$

where

$$Y_o = \text{the oxidation admittance, } \frac{1}{\theta}$$

$$M_o = \text{an oxidation potential, } \frac{M}{L^2}.$$

If the oxidation admittance is defined as

$$Y_o = \frac{K_p}{2M M_o} \quad (3-51)$$

$$\text{and if} \quad M_o \gg M, \quad (3-52)$$

then Equation (3-50) may be rewritten as

$$\frac{dM}{dt} = \frac{K_p}{2M M_o} (M_o - M) \approx \frac{K_p}{2M} \quad (3-53)$$

which is Equation (3-49).

The electrical analog of Equation (3-53) is represented by the network in the following sketch:

3.2.3.3 Oxygen-Uranium Ratios

The amount of oxygen in a fuel node is

$$m = (M) (TSPIN) \quad (3-54)$$

where

m = the amount of oxygen in the node, M

$TSPIN$ = the total surface area of the fuel in the node, L^2 .

In determining the surface area of the fuel, each pellet in a pin was assumed to be a sphere. The volume of a pellet is

$$V = 2\pi a\delta + 2\pi a^2 \quad (3-55)$$

where

a = the pellet radius, L

δ = the pellet thickness, L.

The radius of an equivalent sphere is

$$\alpha = \left(\frac{V}{\frac{4\pi}{3}} \right)^{1/3} \quad (3-56)$$

and the surface area of this sphere is

$$S = 4\pi\alpha^2 \quad (3-57)$$

The total surface area of the fuel in the node then is

$$TSPIN = (S) (N_p) (NPINS) (S'_{node}) \quad (3-58)$$

where

N_p = the number of pellets in a fuel pin,

$NPINS$ = the number of pins per unit area of fuel assembly, and

S'_{node} = the cross-sectional area of fuel assembly in a fuel node.

The oxygen-uranium ratio in a fuel node is

$$\text{Ratio} = \frac{\emptyset}{U} \quad (3-59)$$

where

$\emptyset$ = the number of mass-atoms of oxygen in the fuel node,

U = the number of mass-atoms of uranium in the fuel node.

The number of mass-atoms of oxygen is obtained from Equation (3-60)

$$\emptyset = \frac{M}{AW\emptyset} \quad (3-60)$$

where $AW\emptyset$ = the atomic weight of oxygen.

3.2.3.4 Fuel Oxidation Reaction Rate

It was assumed that the bound up fission gases in the fuel would be released by the oxidation of the UO_2 to U_3O_8 . Assumption of this release mechanism was based on statements made in ORNL-4436 (Reference 25) that

"fission product gases interstitially trapped in oxide fuels can be volatilized and collected in a relatively small volume when these fuels are heated in oxygen at temperatures greater than about 400°C (725°F)."

It was also stated that

". . . the oxidation of UO_2 to U_3O_8 involves a phase change which tends to degrade the oxide³ into a fine granular form."

According to Blackburn, et al.,⁽²⁶⁾ oxidation of UO_2 to U_3O_8 has been observed to occur in two steps. The initial pattern is a smooth parabolic curve from UO_2 to $UO_{2.33}$, where the reaction virtually ceases. The second oxidation stage above $UO_{2.33}$ consists of an induction period, then a stage in which the reaction rate gradually increases, followed by a period in which the speed of reaction tapers off as the composition approaches $UO_{2.67}$. In this study, the parabolic rate law was assumed to hold up to $UO_{2.67}$.

Blackburn further states that the initial oxidation stage is best explained as a diffusion-controlled process, the hypothesis proposed by other authors. He goes on to state, however, that oxygen diffusion is not through the UO_2 structure but through the second phase, U_3O_7 . This reaction is analogous to the diffusion-controlled oxidation of metals where the rate of oxidation is inversely proportional to the oxide thickness.

For spherical particles the parabolic rate equation⁽²⁶⁾ is

$$X = ra \left[1(1-c)^{1/3} \right] = \sqrt{kt} \quad (3-61)$$

where

- X = the thickness of the second phase, L ,
- r = the average radius of the spherical particle, L ,
- a = the ratio of U_3O_7 thickness to UO_2 thickness (approximately 0.99),
- c = the degree of conversion of UO_2 to U_3O_7 ,
- k = the reaction constant, $\frac{L^2}{\theta}$,
- t = the time, θ .

For small values of c , Equation (3-61) reduces to

$$X = \frac{rca}{3} = \sqrt{kt} \quad (3-62)$$

which has already been presented as Equation (3-47).

The square of the slope in the parabolic rate equation gives the reaction constant, k , which varies with temperature. Data on the variation of k with temperature, according to Blackburn, are given in Table 3-7. The heat of activation for the reaction was obtained from an Arrhenius plot. A least squares fit produced the equation

$$\text{Log}_e k = \frac{21700}{RT} - 9.47 \pm 0.15, \quad (3-63)$$

where k is in cm^2/sec , and the heat of activation is 21.7 kcal/mol.

TABLE 3-7

Rate of UO_2 Oxidation from Parabolic Rate Equation
and Experimental Observations

(Reference 26)

Temperature (°C)	$\frac{1}{T} \times 10^3$	k (cm^2/sec)
125(a)	2.512	9.34×10^{-17}
138(a)	2.433	2.79×10^{-16}
160(a)	2.309	9.19×10^{-16}
189	2.164	3.29×10^{-15}
190	2.159	3.88×10^{-15}
200	2.114	6.03×10^{-15}
200	2.114	6.42×10^{-15}
200	2.114	8.02×10^{-15}
210	2.070	1.13×10^{-14}
219	2.032	2.94×10^{-14}
220	2.028	2.01×10^{-14}
231	1.984	3.60×10^{-14}
251	1.908	8.02×10^{-14}
256(b)	1.890	7.88×10^{-14}
270	1.841	1.40×10^{-13}
280	1.808	1.75×10^{-13}
280	1.808	2.32×10^{-13}

(a) Pellet No. 2

(b) Powder

All others are Pellet No. 1.

For the simulation of fuel oxidation, Equation (3-62) was converted to a mass-based rate law in the following manner:

The volume of the spherical particle would be

$$V = \frac{4\pi r^3}{3} \quad (3-64)$$

and the surface area is

$$A = 4\pi r^2. \quad (3-65)$$

The volume-area ratio, then, is

$$\frac{V}{A} = \frac{\frac{4}{3} \pi r^3}{4\pi r^2} = \frac{r}{3} \quad (3-66)$$

which corresponds to the term in Equation (3-62) when $c \approx a \approx 1$.

In terms of the product shell thickness

$$V \approx 4\pi r^2 \chi, \quad (3-67)$$

therefore

$$\frac{V}{A} \approx \frac{4\pi r^2 \chi}{4\pi r^2} = \chi. \quad (3-68)$$

The rate equation defines χ as

$$\chi = \sqrt{kt}. \quad (3-69)$$

Multiplying both sides of the rate equation by $4\pi r^2$ and by the density of the oxidation product gives

$$4\pi r^2 \chi \rho = 4\pi r^2 \rho \sqrt{kt} \quad (3-69)$$

or

$$m = 4\pi r^2 \rho \sqrt{kt}. \quad (3-70)$$

Dividing both sides by $4\pi r^2$ and rearranging, M can be defined as

$$M = \frac{m}{4\pi r^2} = \sqrt{k_p^2 t} \quad (3-71)$$

where

m = the mass of U_3O_7 formed which is equivalent to the mass of oxygen added to the particle, gm,

M = the mass per unit of particle surface area, gm/cm²,

ρ = the density of the oxidation product, $\frac{gm}{cm^3}$.

Let
$$K_p = \rho^2 k, \quad (3-72)$$

therefore
$$M = \sqrt{K_p t}, \quad (3-73)$$

where

K_p = the mass-based rate constant, $\frac{gm^2}{cm^4\text{-sec.}}$

A plot of the mass-based reaction rate constant as a function of temperature is shown in Figure 3-18. The Arrhenius equation was used to extrapolate the experimental data to a temperature of 700°C (1292°F).

3.3 Cask Simulation Networks

The nodal arrangements for the loss-of-coolant models programmed on the Thermal Analyzer Program (TAP) are shown in Figures 3-19, 3-20, and 3-21. Figure 3-19 is the basic heat transfer network for the IF-300 simulation model, which shows the nodes but not how they are connected. This figure relates only the nodes and the dimensions. Figure 3-20 is the complete simulation network of the IF-300 loss-of-coolant model as it is programmed on TAP. This network is actually only a heat transfer network, however, the oxidation and diffusion networks are shown since they were

FIGURE 3-18. Reaction Rate Constant for Oxidation of Uranium Dioxide
(Reference 26)

HEDL 7507-30.7

FIGURE 3-19. Nodal Arrangement for Steady-State and Loss-of-Coolant Models of the IF-300

HEDL 7507-30.9

FIGURE 3-20. Simulation Network of the Loss-of-Coolant Model of the IF-300.

FIGURE 3-21. Idealized Representation of the AMCO Spent Fuel Shipping Cask and Simulation Network of the Loss-of-Coolant Model (Page 1 of 2)

HEDL 7507-30.12

FIGURE 3-21. Idealized Representation of the AMCO Spent Fuel Shipping Cask and Simulation Network of the Loss-of-Coolant Model (Page 2 of 2)

originally part of the model of the conceptual cask design simulated in the early stages of the study. The IF-300 model includes some new features which this early model did not have, but the oxidation and diffusion networks were not needed so they were not retained. However, these networks may be added later if desired. Network interactions, switching, and other functions of the central processor are not shown, but some of these have been discussed earlier and will be discussed further and illustrated in the next section. In Figure 3-20, the circled numbers identify only nodes. The admittances are also numbered since some are referred to in the following sections. Figure 3-21 is the simulation network of the loss-of-coolant model of the AMCO cask. It consists of only the heat transfer network. The oxidation and diffusion networks are omitted. In this figure, as in Figure 3-20, the node numbers are circled, and the admittance numbers are not circled. The central processor in TAP also controls the network interactions, switching and other functions for this network.

3.4 Central Processor: Control of Thermal Radiation, Melting and Fuel Oxidation

Algorithms controlling switching, melting, oxidation, and interactions of the three networks are functions of the central processor.

3.4.1 Thermal Radiation

In Figure 3-20, connectors 3, 4, 6, 10, 12, 24, 25, and 28 are thermal radiation admittances. Admittances 3 and 10 represent radiation heat transfer paths from the outer row of pins in the fuel assemblies to the inside of the assembly cans. Admittance 6 is a composite connector representing heat flow by conduction in the outer fringes of the fuel assembly, and radiation to the assembly can. Heat transfer between the inner fuel assembly and the outer fuel assemblies is represented by admittance 4. Admittances 12 and 25 are the radiation paths from the outer fuel assemblies and the inner fuel assembly, respectively, to the inner surface of the cask cavity. Thermal radiation across the outer water jacket is represented by admittance 24, and radiation from the outer surface of the jacket to the surroundings by admittance 28.

Thermal radiation is computed automatically by the TAP code central processor, based on the following development of an expression for the thermal radiation admittance.

The heat transferred from node $(m + 1)$ to node m is

$$Q = \sigma A^F (T_{m+1}^4 - T_m^4) \quad (3-74)$$

where

- T_m = the absolute temperature of the m -th node, T ,
- σ = the Stefan-Boltzmann constant, $H/\theta T^4 L^2$,
- F = the combination emissivity and shape factor,
- A = the surface area for radiation, L^2 .

If Equation (3-74) is rewritten as

$$Q = h_r A^F (T_{m+1} - T_m) \quad (3-75)$$

then the coefficient for heat transfer by radiation, h_r , is

$$h_r = \sigma \left(\frac{T_{m+1}^4 - T_m^4}{T_{m+1} - T_m} \right) \quad (3-76)$$

or

$$h_r = \sigma \left(T_{m+1}^3 + T_m T_{m+1}^2 + T_m^2 T_{m+1} + T_m^3 \right) . \quad (3-77)$$

Defining a radiation admittance, Y_R , as

$$Y_R = h_r A^F , \quad (3-78)$$

and substituting from Equation (3-77),

$$Y_R = \sigma A F \left(T_{m+1}^3 + T_m T_{m+1}^2 + T_m^2 T_{m+1} + T_m^3 \right) . \quad (3-79)$$

The central processor automatically computes values of Y_R to be used between nodes m and $m+1$ in the heat transfer network, based on temperatures from the previous iteration.

The combination emissivity and shape factor is expressed as

$$F = F_A F_\epsilon \quad (3-80)$$

where

F_A = the geometric view factor or shape factor,
 F_ϵ = the emissivity factor.

The emissivity factor used is given by the expression

$$F_\epsilon = \frac{1}{\frac{1}{\epsilon_{m+1}} + \frac{1}{\epsilon_m} - 1} \quad (3-81)$$

where

ϵ_m = the emissivity of the radiating m -th node.

Approximate shape factors were used for all radiation paths except those at the outer water jacket and finned surfaces. View factors for a finned cylindrical surface are shown in Figure 3-22.⁽²⁷⁾

3.4.2 Melting

In the opening paragraphs of the Appendix it was pointed out that the IF-300 was not modeled until the final stages of the study. The LWR spent fuel shipping cask modeled and studied throughout most of the study was a conceptual design that was never actually built. One of the important differences between this cask and the IF-300 is the type of gamma shielding used. The conceptual design is lead-shielded. The IF-300 shield is depleted uranium.

$$F_{G_1 - \infty} = 0.17$$

$$F_{G_2 - \infty} = 0.18$$

$$F_{G_1 - 1} = 0.69$$

$$F_{G_2 - 2} = 0.00$$

$$F_{G_1 - 2} = 0.14$$

$$F_{G_2 - 1} = 0.42 \times 2^*$$

$$\sum F_G = 1.00$$

$$\sum F_G = 1.00$$

*NOTE THAT THE CYLINDER SEES TWO FINS SIMULTANEOUSLY

HEDL 7507-30.17

FIGURE 3-22. Geometric View Factors for a Typical Fin-Cylinder Cavity (Reference 27)

The simulation network of the loss-of-coolant model of the conceptual cask included circuitry and logical switches to simulate melting of the lead shield during a fire. Since the model of this cask has been preserved for possible future use to evaluate the behavior of casks designed with lead shields, a brief discussion of the techniques used to simulate melting of the lead shield will be presented.

Two sets of admittances are used to represent the lead shield, as shown in the following sketch. The admittance labeled Y_A represents heat conduction in the lead between nodes 17 and 18. The admittance labeled Y_B represents heat transfer by radiation from the outer steel shell, node 21, and the lead node 17, across the void space created when lead nodes 18, 19 and 20 melt away.

These thermal radiation and conduction admittances for the lead shield are activated by logical switches and are switched in and out of the circuit as the appropriate nodes reach the melting temperature of the lead, absorb the latent heat of melting, and melt or ablate away. Algorithms for controlling the switching of these admittances are shown in Figures 3-23 and 3-24.

HEDL 7507-30.19

FIGURE 3-23. Algorithm for Controlling Latent Heat of Melting

HEDL 7507-30.20

FIGURE 3-24. Algorithm for Controlling the Switching of Admittances Simulating Melting

In Figure 3-23, the node temperature is compared to the melting temperature of the node material. If the node temperature, T_m , is less than the melting temperature, MP_m , computation of the node temperature is continued as part of the network computations. If the node temperature is equal to the melting temperature, the node temperature is held equal to the melting temperature and the heat input to the node is integrated over time. The latent heat, H_m , for the node is precalculated and entered as input. This is a particular value depending upon the mass of material in node "m". The integrated heat to the node is compared to the latent heat for the node and, if it is equal to or greater than the latent heat, the computation of T_m progresses as part of the regular network computations. If the integrated heat is less than the latent heat for the node, the algorithm returns the progress of the computations to the point where the node temperature is being held equal to the melting temperature, and the heat input is integrated again to complete the cycle.

Figure 3-24 shows how the node temperature is used to activate the switching circuits. First of all, 0.2 of a degree, a very small arbitrarily selected temperature rise, is added to the melting point of the node. This is designated as TMP_m , a temperature slightly higher than the melting temperature. The node temperature T_m is then compared to TMP_m and, if it is greater than or equal to TMP_m , node "m" is disconnected from the network. Also, two switching variables, D1 and D2, are set either equal to zero or to one, depending upon whether the node temperature is equal to or greater than TMP_m , or whether it is less than TMP_m . When the node temperature is greater than the melting temperature, $D1 = 1$, and $D2 = 0$. If the node temperature is less than the melting temperature, $D1 = 0$, $D2 = 1$, and node "m" is not disconnected from the network. The affected admittances are then multiplied by D1 and D2 and inserted into the heat transfer network.

3.4.3 Fuel Oxidation

The algorithm in the central processor that controls the switching process simulating the release of the "bound up" fission gases by oxidation of the fuel is shown in Figure 3-25. This algorithm is an illustration of how interactions of the heat transfer, oxidation and diffusion networks are controlled by the central processor.

In Figure 3-25, the mass gain per unit surface area of fuel in node m due to oxidation, M_m , from the oxidation network is converted to the mass of oxygen, m_m , by multiplying by the total surface area of fuel in the node, $TSPIN_m$ [see Equation (3-54)]. The mass of oxygen is then divided by the atomic weight of oxygen, AWO , to obtain the number of mass atoms, ϕ_m [Equation (3-60)]. The oxygen-uranium ratio for the node, $(\frac{\phi}{U})_m$, is then determined by dividing ϕ_m by the number of mass-atoms of uranium in the node, U_m [Equation (3-59)]. This ratio is compared to the ratio, $(\frac{\phi^{PD}}{U})_m$, which bounds the U_3O_8 region on a UO_2 - U_3O_8 phase diagram (see Figure 3-26). $(\frac{\phi^{PD}}{U})_m$ is a function of the node temperature, T_m , which is obtained from the heat transfer network. The decision block in the algorithm of Figure 3-25 compares the node ratio $(\frac{\phi}{U})_m$ with the phase diagram ratio, $(\frac{\phi^{PD}}{U})_m$. A switching variable, $D4$, is set either equal to zero or to one, depending upon whether or not $(\frac{\phi}{U})_m$ is greater than or equal to $(\frac{\phi^{PD}}{U})_m$. When $(\frac{\phi}{U})_m \geq (\frac{\phi^{PD}}{U})_m$, $D4 = 1$, and when $(\frac{\phi}{U})_m < (\frac{\phi^{PD}}{U})_m$, $D4 = 0$. The number of moles of bound up fission gases in the node, N_m , from the diffusion network, is multiplied by $D4$ and becomes GS_m , the number of moles released from node m . GS_m is then multiplied by the factor C/M , which is the number of curies radioactivity per mole, to give CG_m , the number of curies radioactivity in the bound up gases released.

The PWR fuel is UO_2 , while the FFTF or LMFBR-type fuel is UO_2 - PuO_2 . It was assumed that the bound up fission gases would be released from the LMFBR-type fuel when the UO_2 in the fuel oxidizes to U_3O_8 , even though PuO_2 is present. The UO_2 - U_3O_8 phase diagram used for the PWR fuel (Figure 3-26) is assumed to be valid for the LMFBR-type fuel. The oxygen-uranium ratios that bound the U_3O_8 regions on this phase diagram are compared to the calculated ratios for both types of fuel to signal the conversion of UO_2 to U_3O_8 .

FIGURE 3-25. Algorithm Controlling the Simulation of the Release of "Bound Up" Fission Gases

FIGURE 3-26. Phase Diagram for Oxides of Uranium (Reference 31)

Figure 3-27 is a typical portion of the logic control and information flow of the processor in both loss-of-coolant models. Melting and switching algorithms for the lead in the conceptual cask, and controlling algorithms for monitoring the failure of the fuel pin clads and for the release of bound-up fission gases in both type casks are shown.

3.5 Proposed Modifications to Loss-of-Coolant Models to Simulate the Flow of Fission Gases and Residual Coolant Vapor from the Casks

Two breach sizes were evaluated, using the coolant loss rate models discussed in Section 2, to determine the rate at which the primary coolant is lost from the casks. After the primary coolant is lost, the fuel assembly temperatures will rise and the free fission gases in the pins will expand. Some of the fuel pins will reach temperatures high enough for the expanding fission gases to cause clad failure, releasing the fission gases to the cask containment. The events leading up to fission gas release and the mechanisms of release have already been discussed earlier in Section 3. Once the fission gases are released to the cask containment, they would mix with the residual coolant vapor, and the mixture could flow from the cask through the breach, just as the primary coolant did earlier in the sequence of events.

A system of equations was developed to define the rate of flow of fission gases and volatile solids from a cask. This system of equations was developed too late for modification of the present loss-of-coolant models and volatile solids release model. However, some of the equations will be derived and discussed here. Additional equations necessary for modification of the volatile solids release model will be presented and discussed in Section 4.

3.5.1 Mass Balance on the Cask Containment

A mass balance on the cask cavity, in terms of moles of fission gases, can be written as

HEDL 7507-30.24

FIGURE 3-27. Typical Portion of the Logic and Information Control of the Processor (Page 1 of 7)

HEDL 7507-30.25

FIGURE 3-27. Typical Portion of the Logic and Information Control of the Processor (Page 2 of 7)

FIGURE 3-27. Typical Portion of the Logic and Information Control of the Processor (Page 3 of 7)

HEDL 7507-30.27

FIGURE 3-27. Typical Portion of the Logic and Information Control of the Processor (Page 4 of 7)

HEDL 7507-30.28

FIGURE 3-27. Typical Portion of the Logic and Information Control of the Processor (Page 5 of 7)

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FIGURE 3-27. Typical Portion of the Logic and Information Control of the Processor (Page 7 of 7)

$$\left[\begin{array}{l} \text{Rate of Change of} \\ \text{Moles of Fission} \\ \text{Gases in the Cask} \\ \text{Cavity} \end{array} \right] = \left[\begin{array}{l} \text{Rate of release} \\ \text{of Fission Gases} \\ \text{to the Cavity} \\ \text{From the Fuel} \end{array} \right] - \left[\begin{array}{l} \text{Rate of loss of} \\ \text{Fission Gases} \\ \text{from the Cavity} \\ \text{by Leakage} \end{array} \right]$$

or

$$\frac{dm}{dt} = \sum_{k=1}^K \delta_k(t) m_k - \frac{\mu u A_{GAP}}{V_{CSK} f_m} \quad (3-82)$$

$$(k=1, \dots, K)$$

where

- m = the number of moles of fission gases in the cask, lb-moles,
- m_k = the number of moles of fission gases in the k -th fuel node, lb-moles,
- A_{GAP} = the cross-sectional area of the breach opened in the cask containment, in²,
- V_{CSK} = the free volume inside the cask, in³,
- u = the velocity at which the gas mixture flows through the breach, in/sec,
- $\delta_k(t)$ = the Dirac impulse function applicable to the k -th fuel node, 1/sec,
- f_m = the mole fraction of fission gases in the mixture of residual coolant vapor and fission gases.

The first term on the right hand side of Equation (3-82) is a source term, and the second term is the leakage term.

The source term is based on known values of m_k and the release times for the k fuel nodes as obtained from results from the loss-of-coolant models. At the time the pin clads burst in fuel node k , the impulse function $\delta_k(t) = 1$. Before and after this burst time, $\delta_k(t) = 0$.

The leakage term is based on the volumetric rate of flow of fission gases from the cask, and the number of moles in a unit volume of fission gases. The flow velocity u was determined from an energy balance on the breach.

3.5.2 Energy Balance on the Breach: Determination of Flow Velocity

The First Law of Thermodynamics states that the total energy change in a system is equal to the difference between the heat added to the system and the work done by the system. This is expressed as Equation (3-83)

$$dE = J\delta Q - \delta w \quad (3-83)$$

where

- dE = the change in the total energy in the system, F-L/M,
- δQ = the heat added to the system, H/M,
- δw = the work done by the system, F-L/M,
- J = the mechanical equivalent of heat, F-L/H.

In terms of the various forms of energy included in the total energy of the system, the energy balance for a unit mass of fluid flowing may be written as

$$Jde + d\left(\frac{P}{\rho}\right) + d\left(\frac{u^2}{2g_c}\right) + \frac{gdZ}{g_c} = J\delta Q - \delta w \quad (3-84)$$

where

- de = the change in the internal energy of the fluid, H/M,
- $d\left(\frac{P}{\rho}\right)$ = the change in the flow work of the fluid, F-L/M,
- ρ = the fluid density, M/L³.
- $d\left(\frac{u^2}{2g_c}\right)$ = the change in the kinetic energy of the fluid, F-L/M,
- dZ = the change in the height (potential energy) of the fluid, L
- g = the local acceleration of gravity, L/θ²,
- g_c = the gravitational constant, ML/Fθ².

Considering the unit mass of fluid as if it were at rest, the internal energy term may be obtained from the First Law for a non-flow process,

$$Jde = J\delta Q_T - Pd\left(\frac{1}{\rho}\right), \quad (3-85)$$

where

δQ_T = the total thermal effects from all sources, H/M

$Pd\left(\frac{1}{\rho}\right)$ = a term representing all compression effects, F-L/M.

Since δQ_T represents the total thermal effects from all sources, it may be written as

$$\delta Q_T = \delta Q + \delta F \quad (3-86)$$

where

δF = the energy added to the fluid due to friction, H/M.

Substituting from (3-85) and (3-86) into (3-84), the total energy balance becomes

$$J\delta Q + J\delta F - pd\left(\frac{1}{\rho}\right) + d\left(\frac{P}{\rho}\right) + d\left(\frac{u^2}{2g_c}\right) + \frac{gdZ}{g_c} = J\delta Q - \delta w \quad (3-87)$$

$$\text{or} \quad J\delta Q + J\delta F - pd\left(\frac{1}{\rho}\right) + Pd\left(\frac{1}{\rho}\right) + \frac{1}{\rho} dP + d\left(\frac{u^2}{2g_c}\right) + \frac{gdZ}{g_c} = J\delta Q - \delta w. \quad (3-88)$$

Since the potential energy of the gas is negligible, and since no work is done by the system, Equation (3-88) may be reduced to

$$-\frac{1}{\rho} dP = J\delta F + d\left(\frac{u^2}{2g_c}\right). \quad (3-89)$$

Assuming an average gas density, Equation (3-89) may be integrated across the breach to give

$$-\frac{1}{\rho} (P_{ATM} - P_{CSK}) = J\Delta F + \frac{u^2 - u_{CSK}^2}{2g_c} \quad (3-90)$$

where

P_{CSK} = the pressure inside the cask, F/L^2

P_{ATM} = the pressure outside the cask, F/L^2

u_{CSK} = the velocity of the gas inside the cask, L/θ .

Since $u_{CSK} \approx 0$

then Equation (3-90) becomes

$$P_{CSK} - P_{ATM} = \rho J \Delta F + \rho \frac{u^2}{2g_c} \quad (3-91)$$

or

$$P_{CSK} - P_{ATM} = \Delta P_F + \rho \frac{u^2}{2g_c} \quad (3-92)$$

where

ΔP_F = the pressure drop due to frictional effects, F/L^2 .

The pressure drop, ΔP_F , is the sum of the frictional losses of mechanical energy due to:

1. The contraction of the fluid at the entrance to the breach (entrance loss),
2. The flow of the fluid in the breach, and
3. The expansion of the fluid at the outlet of the breach (exit loss).

The entrance loss may be expressed as Equation (3-93) ⁽²⁸⁾

$$\Delta P = 0.4\rho \left(1.25 - \frac{A_{GAP}}{S_{CSK}} \right) \frac{u^2}{2g_c} \quad (3-93)$$

where

S_{CSK} = the area of the inside surface of the cask, L^2 .

The loss in the breach is defined by the Fanning equation⁽²⁸⁾

$$\Delta P = \frac{4 \rho f L_{GAP} u^2}{2 g_c D_{GAP}} \quad (3-94)$$

where

L_{GAP} = the length of the flow passage represented by the breach, L ,

D_{GAP} = the equivalent diameter of the breach, L

f = the Fanning friction factor.

For small Reynolds numbers ($R_e = \frac{D u \rho}{\mu}$), the Fanning friction factor may be expressed as

$$f = \frac{16 \mu}{D_{GAP} u \rho} \quad (3-95)$$

where

μ = the absolute viscosity of the fluid, $\frac{M}{\theta L}$.

Substituting from Equation (3-95) into (3-94), the pressure loss in the breach may be expressed as

$$\Delta P = \frac{32 \mu L_{GAP} u}{D_{GAP}^2 g_c} \quad (3-96)$$

The exit loss is defined as⁽²⁸⁾

$$\Delta P = \frac{\rho u^2}{2g_c} \left(1 - \frac{A_{GAP}}{S_o} \right)^2 \quad (3-97)$$

where

S_o = the cross-sectional area of the outlet region, L^2 .

Adding Equations (3-93), (3-96) and (3-97) and substituting the results into the energy balance [Equation (3-92)] gives

$$\begin{aligned} P_{CSK} - P_{ATM} = & 0.4\rho \left(1.25 - \frac{A_{GAP}}{S_{CSK}} \right) \frac{u^2}{2g_c} + \frac{32\mu L_{GAP} u}{D_{GAP}^2 g_c} \\ & + \frac{\rho u^2}{2g_c} \left(1 - \frac{A_{GAP}}{S_o} \right)^2 + \frac{\rho u^2}{2g_c} . \end{aligned} \quad (3-98)$$

Now $S_{CSK} \gg A_{GAP}$,

and $S_o \gg A_{GAP}$,

therefore Equation (3-98) may be reduced to

$$P_{CSK} - P_{ATM} = 2.5 \frac{\rho u^2}{g_c} + \frac{32\mu L_{GAP} u}{D_{GAP} g_c} \quad (3-99)$$

It can be shown that the first term on the right hand side of Equation (3-99) is a small fraction of the second term and may be neglected. Therefore, the fluid velocity may be expressed as

$$u = \frac{D_{GAP}^2 g_c (P_{CSK} - P_{ATM})}{32\mu L_{GAP}} . \quad (3-100)$$

The pressure in the cask may be determined using the gas law

$$P_{CSK} = \frac{m R T_{CSK}}{V_{CSK} f_m} , \quad (3-101)$$

where

R = the universal gas constant, L-F/T-Mole

T_{CSK} = the absolute temperature of the mixture of residual coolant vapor and fission gases in the cask, T.

Substituting this into Equation (3-100) gives

$$u = \frac{D_{GAP}^2 g_c \left(\frac{m R T_{CSK}}{V_{CSK} f_m} - P_{ATM} \right)}{32\mu L_{GAP}} . \quad (3-102)$$

The mass balance [Equation (3-82)] may now be written as

$$\frac{dm}{dt} = \sum_{k=1}^K \delta_k(t) m_k - \frac{m A_{GAP} D_{GAP}^2 g_c \left(\frac{m R T_{CSK}}{V_{CSK} f_m} - P_{ATM} \right)}{32\mu L_{GAP} V_{CSK} f_m} \quad (3-103)$$

$$\frac{dm}{dt} = \sum_{k=1}^K \delta_k(t) m_k - \frac{A_{GAP} D_{GAP}^2 g_c}{32\mu L_{GAP} V_{CSK} f_m} \left(\frac{R T_{CSK} m^2}{V_{CSK} f_m} - P_{ATM} m \right) \quad (3-104)$$

or
$$\frac{dm}{dt} = \sum_{k=1}^K \delta_k(t) m_k - Am^2 + Bm \quad (3-105)$$

where
$$A = \frac{A_{GAP} D_{GAP}^2 g_c R T_{CSK}}{32\mu V_{CSK}^2 L_{GAP} f_m^2} \quad (3-106)$$

and
$$B = \frac{A_{GAP} D_{GAP}^2 g_c P_{ATM}}{32\mu V_{CSK} L_{GAP} f_m} \quad (3-107)$$

The equivalent diameter of the breach is defined as

$$D_{GAP} = \frac{4A_{GAP}}{P_W} \quad (3-108)$$

where

P_W = the wetted perimeter, L.

The wetted perimeter is obtained from

$$P_W = 2\pi D \quad (3-109)$$

where

D = the mean diameter of the cask wall, L.

3.5.3 Proposed Modifications to the Loss-of-Coolant Models

To modify the present loss-of-coolant models to simulate the flow of fission gases from the cask through the breach to the surroundings, the following changes would be required.

1. Another network, similar to the oxidation and diffusion networks, would have to be added to represent the fission gas mass balance on the cask containment [Equation (3-82)]. Also, the additional equations defining the flow velocity would have to be included in the central processor.
2. The pressure and temperature of the mixture of fission gases and residual coolant vapor in the cask containment would have to be determined. This would be done by treating the mixture as a coolant, using the same techniques discussed in Section 2.

3.5.3.1 Fission Gas Leakage Network

The fission gas mass balance on the cask containment is defined by Equation (3-82). This equation may be revised to express the loss or leakage term as a mass transfer term as shown in Equation (3-110),

$$\frac{dm}{dt} = \sum_{k=1}^K \delta_k(t) m_k - Y_L (m - m_0) \quad (3-110)$$

where

$$\begin{aligned} m_0 &= \text{the number of moles of fission gases in the surroundings,} \\ &\quad \text{lb-moles} \\ \text{and } Y_L &= \text{a fission gas leakage admittance, } 1/\theta, \\ &= \frac{u A_{GAP}}{V_{CSK}}. \end{aligned} \quad (3-111)$$

The electrical analog of Equation (3-110) is shown in the following sketch.

The capacitance of the node representing the number of moles of fission gases in the cask containment is equal to 1.0. The sink node is represented by m_0 , which would be assumed to be approximately equal to 0 since the escaping fission gases will be dispersed and the concentration would be negligible. The switches in the network represent the Dirac impulse functions, δ_k . These switches would be equivalent to the switch D3 in the algorithm of Figure 3-16, which is already programmed into the central processor.

3.5.3.2 Gas Mixture in Cask Containment as a Coolant: Determination of Temperature and Pressure

The velocity in the leakage term of Equations (3-82) and (3-111) is a function of the pressure of the mixture of fission gases and residual coolant vapor in the cask, as shown in Equation (3-100). Equation (3-101) states that the pressure is, in turn, a function of the temperature of the mixture. This suggests that the loss-of-coolant models must treat this mixture as a coolant. This would be no problem since the residual coolant vapor left in the cask after loss of the coolant is already treated as a coolant.

The volumetric heat dissipation admittances would be determined as outlined in Sections 1.2, 2.1.1.3.1, and 3.1.2, except that the mixture of fission gases and residual coolant vapor would be the coolant.

The apparent thermal conductivity would be determined as outlined in Section 3.1.3 except that, instead of residual coolant vapor, a mixture of fission gases and vapor would be the heat transfer medium.

3.5.3.3 Fission Gases in Cask Containment as a Deterrent to Fuel Pin Clad Failure

Fission gases released to the cask containment from the first fuel pins to burst will tend to oppose the bursting of additional pins. As the released fission gases are heated, the pressure in the cask containment will rise. This would decrease the differential pressure across the remaining fuel pin clads, which would delay their failure.

The increased pressure in the cask would only delay clad failure and further release of fission gases, not prevent it. As the fuel temperatures increase with time, the internal pressures in the pins will increase and the strength of the clads will decrease. During the same time interval, some of the fission gases already released to the cask containment will have leaked from the cask through the breach. This would tend to relieve the pressure in the cask. The net result would be a rise in the differential pressure across the fuel pin clads, some of which would eventually fail. Whenever any of the pins fail, the events outlined above would be repeated. The effect of the pressure in the cask on pin clad failure is evident upon examination of the hoop stress formula presented earlier as Equation (3-19),

$$\frac{\Delta P}{S} = \frac{2 (R_o - 1)}{(R_o + 1)} , \quad (3-19)$$

where ΔP is the differential pressure across the fuel pin clads. This equation shows that the stress on the clads is directly proportional to the differential pressure.

3.5.3.4 Choked Flow of Gas Mixture in the Breach: Determination of Sonic Velocity

Fission gases and residual coolant vapor are compressible. Consequently, the flow of these gases through the breach must be checked to determine if the flow is choked. The flow would be choked if the gas velocity is equal to (or greater than) the velocity of sound in the gas, i.e., the Mach number would be equal to 1.0. Although it is felt that the flow would be substantially less than sonic, it should be checked because, if it is choked, the pressure in the cask would rise to higher levels. This would further prevent or delay failure of the pin clads.

Although the flow term in the mass balance equation [Equation (3-82)] was based on an energy balance which was not restricted to isentropic flow, the equations used to check for choked flow are based on an energy balance on the gas assuming it is flowing isentropically through the breach. This energy balance may be expressed as

$$h_o = h + \frac{u^2}{2g_c} \quad (3-112)$$

where

h = the enthalpy of a unit mass of gas flowing in the breach, F-L/M,
 h_o = the enthalpy of a unit mass of gas in the cask, F-L/M.

Assuming the gas behaves as a perfect gas, Equation (3-112) may be rewritten as

$$C_p T_o = C_p T + \frac{u^2}{2g_c} \quad (3-113)$$

where

C_p = the specific heat of the gas at constant pressure, F-L/MT
 $T_o = T_{CSK}$ = the absolute temperature of the gas in the cask, T,
 T = the absolute temperature of the gas flowing in the breach, T.

Using the following definitions

$$\gamma = \frac{C_p}{C_v} \quad (3-114)$$

and $R = C_p - C_v \quad (3-115)$

where

C_v = the specific heat of the gas at constant volume, F-L/MT

and R = the specific gas constant for the gas, F-L/MT,

C_p may be expressed as

$$C_p = \frac{\gamma R}{\gamma - 1} \quad (3-116)$$

Substituting Equation (3-116) into (3-113), and rearranging gives

$$\frac{T_o}{T} = 1 + \frac{(\gamma - 1)}{2} \frac{u^2}{g_c \gamma R T} \quad (3-117)$$

The definition of the velocity of sound in an ideal gas at temperature T is

$$a = \sqrt{g_c \gamma R T} \quad (\text{Reference 29, p. 643}) \quad (3-118)$$

Substituting Equation (3-118) into (3-117) yields

$$\frac{T_o}{T} = 1 + \frac{(\gamma - 1)}{2} \frac{u^2}{a^2} \quad (3-119)$$

and, since the Mach number is defined as

$$M = \frac{u}{a} \quad (3-120)$$

Equation (3-119) becomes

$$\frac{T_o}{T} = 1 + \frac{(\gamma-1)M^2}{2} \quad (3-121)$$

or

$$T = T_o \left[1 + \frac{(\gamma-1)M^2}{2} \right]^{-1} \quad (3-122)$$

If the flow is choked, the Mach number would be 1.0, so Equation (3-122) would reduce to

$$T = T_o \left[1 + \frac{(\gamma-1)}{2} \right]^{-1} \quad (3-123)$$

Substituting Equation (3-123) into (3-118) gives

$$a = \sqrt{g_c \gamma R T_o \left[1 + \frac{(\gamma-1)}{2} \right]^{-1}} \quad (3-124)$$

which is compared to the value of u computed during the transient. If $u < a$, the flow is not choked.

3.5.3.5 Relationship of Gas Leakage to Volatile Solids Release Models

The proposed changes to the Loss-of-Coolant models, to simulate the flow of gas mixture from the casks, will allow modifications to be made to the Volatile Solids Release Models to determine the amount of volatile solids that may flow through the breach opened in the cask containment.

The modifications developed in Section 3.5 will allow determination of the velocity of the gas mixture flowing from the gap [see Equation (3-102)]. This velocity is the key variable in the development of a proposed term representing the removal of particles from an aerosol in the cask by leakage through the breach. This removal term will be added to the particle

balance equation [Equation (4-44)] of Section 4.1.4. The derivation of this term and the procedure for adding it to the present Volatile Solids Release models are presented in Section 4.1.5.

4. MODEL SIMULATING BEHAVIOR OF VOLATILE SOLIDS OR SOLID FISSION PRODUCTS RELEASED FROM DAMAGED SPENT FUEL IN A CASK

A model was devised to simulate the behavior of volatile solids or solid fission products (cesium compounds) released as an aerosol to the containment vessel or cavity in a spent fuel shipping cask following an accident, fire and loss of primary coolant. The purpose of the volatile solids release model (VSOL) development was to provide a tool to estimate the amount of volatile solids or solid fission products that would be suspended in the cask containment as an aerosol. The amount in suspension as an aerosol represents the amount that could potentially be released from the containment to the surroundings. Proposed modifications to the model to include a leakage term are presented in Section 4.1.5. This term will represent the flow of volatile solids from the breach opened in the cask at impact.

The volatile solids release model is a system of equations derived in this section. These equations were programmed for simulation using MIMIC, a continuous system simulation program. A calculation control flow diagram of the model is presented as Figure 4-1, and the MIMIC listing is presented as Figure 4-2.

4.1 Coagulation Equation - A Particle Balance Equation for Aerosols

The model VSOL was based on the basic coagulation equation for aerosols having a distribution of particle sizes, modified to include terms for particle removal or loss to the system and a source term⁽¹²⁾:

$$\frac{\partial n}{\partial t} (v,t) = A_+ (v,t) - A_- (v,t) - R (v,t) + S (v,t) \quad (4-1)$$

where

$n(v,t)$ = the concentration of particles of volume v ,
particles/cm³ of aerosol

$A_+(v,t)$ = the rate of formation of particles of volume v
by agglomeration of smaller particles, par-
ticles/cm³ (aerosol) x sec.

HEDL 7507-30.36

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 1 of 10)

HEDL 7507-30.37

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 2 of 10)

HEDL 7507-30.38

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 3 of 10)

HEDL 7507-30.39

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 4 of 10)

HEDL 7507-30.40

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 5 of 10)

HEDL 7507-30.41

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 6 of 10)

HEDL 7507-30.42

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 7 of 10)

HEDL 7507-30.43

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 8 of 10)

HEDL 7507-30.44

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 9 of 10)

HEDL 7507-30.45

FIGURE 4-1. Calculation Control Flow Diagram of the Volatile Solids Release Model of the IF-300 Spent Fuel Shipping Cask (Page 10 of 10)

VSOL - A MODEL SIMULATING THE TRANSIENT BEHAVIOR OF THE VOLATILE SOLIDS
 RELEASED AS AN AEROSOL WHEN THE FUEL PINS BURST FOLLOWING LOSS
 OF PRIMARY COOLANT FROM THE IF-300 SPENT FUEL SHIPPING CASK.

***** THIS MODEL IS PROGRAMMED IN A LANGUAGE FOR MIMIC, A CONTINUOUS
 SYSTEM SIMULATION PROGRAM *****

NOMENCLATURE OF TERMS *****

ACTNM = ACTIVITY OF A PARTICLE WITH RADIUS RNM (N=1,,5)(M=N+1),
 CURIES/PARTICLE
 ACTVTY = TOTAL ACTIVITY OF ALL THE PARTICLES REMAINING IN
 SUSPENSION AS AN AEROSOL IN THE CASK, CURIES
 ASURF = SURFACE AREA BOUNDING AEROSOL UPON WHICH PLATEOUT MIGHT
 OCCUR, CM**2
 ATNM = TOTAL ACTIVITY OF PARTICLES IN THE SIZE RANGE RN TO RM
 RELEASED FROM ALL X FUEL NODES (SUM OF FREE AND BOUND-UP)
 (X=1,,10, CURIES
 ATOT = TOTAL ACTIVITY OF PARTICLES IN ALL SIZE RANGES RELEASED
 FROM ALL X FUEL NODES (SUM OF FREE AND BOUND-UP)(X=1,,10),
 CURIES
 BLDELT = THICKNESS OF BOUNDARY LAYER BETWEEN AEROSOL AND BOUNDING
 SURFACES, ASURF, UPON WHICH PLATEOUT MIGHT OCCUR, CM
 BSWJ = LOGICAL CONTROL VARIABLE (LCV), FUNCTION SWITCH. BSWJ=1.
 WHEN TIME.GE.TBJ, AND BSWJ=0. WHEN TIME.LT.TBJ (J=1,,10),
 BURST SWITCH.
 CDN = COMBINED SETTLING AND PLATEOUT TERM COEFFICIENTS (N=1,,5)
 (M=N+1), 1/SEC
 CHCK = LOGICAL CONTROL VARIABLE (LCV), FUNCTION SWITCH. TRUE OR
 ON IF SNOOP.GT.0., OFF OTHERWISE. THIS LCV USED FOR
 SELECTED OPTIONAL PRINTOUT.
 CNM = SETTLING TERM COEFFICIENTS (N=1,,5)(M=N+1), 1/SEC
 CPM = THE NUMBER OF CURIES IN A GRAM OF VOLATILE SOLID, CI/GM
 CSC = ARRAY NAME. CUNNINGHAM SLIP COEFFICIENTS VS PARTICLE
 RADIUS.
 CSCNM = CUNNINGHAM SLIP COEFFICIENTS FOR EACH PARTICLE SIZE GROUP
 (N=1,,5)(M=N+1)
 DC = INSIDE DIAMETER OF CAVITY, CM
 DCOF = CASK SHAPE FACTOR FOR PLATEOUT TERMS, 1/CM**2
 DIFCOF = ARRAY NAME. PLATEOUT DIFFUSION COEFFICIENTS VS PARTICLE
 RADIUS.
 DLTR = RANGE OF RADII IN EACH PARTICLE SIZE GROUP (INCREMENT OF
 PARTICLE SIZE RANGE), CM
 DNM = PLATEOUT TERM COEFFICIENTS (N=1,,5)(M=N+1), 1/SEC
 DPNM = COEFFICIENT FOR DIFFUSION OF PARTICLES OF RADIUS RNM
 THROUGH BOUNDARY LAYER BETWEEN AEROSOL AND BOUNDING
 SURFACES (N=1,,5)(M=N+1), CM**2/SEC

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
 for the IF-300 (Page 1 of 16)

DT = TIME STEP FOR PRINTOUT, SECONDS
 DX = DIAMETER OF EXPANSION CHAMBER, CM
 ETA = VISCOSITY OF ATMOSPHERE IN CASK, GM/SEC-CM
 FACT = CORRECTION FACTOR TO ADJUST THE NUMERICAL COEFFICIENT OF
 THE SELF-PRESERVING DISTRIBUTION FUNCTION IN SUBPROGRAM
 NMBR TO GIVE CORRECT MASS AND ACTIVITY.
 FCSK = CASK SHAPE FACTOR FOR SETTLING TERMS, 1/CM
 (SETTLING OUT SURFACE/FREE VOLUME INSIDE CASK)
 FG = THE FRACTION OF FISSION GASES WHICH HAS
 MIGRATED TO THE PIN VOID DURING REACTOR OPERATION
 FR = THE FRACTION OF SOLIDS RELEASED FROM THE PINS
 FSOL = THE FRACTION OF SOLIDS WHICH HAS MIGRATED TO THE PIN VOIDS DURING
 REACTOR OPERATION
 G = ACCELERATION DUE TO GRAVITY, CM/SEC**2
 HOURS = TIME, HOURS
 ITERAT = LOGICAL CONTROL VARIABLE (LCV), FUNCTION SWITCH. TRUE OR
 ON WHEN ABS(MTOTIN-MTOT).GT.1., OFF OTHERWISE.
 LOSSNM = RATE OF LOSS OF PARTICLES, IN SIZE RANGE RN TO RM, FROM
 AEROSOL DUE TO SETTLING AND PLATEOUT (TIME DERIVATIVE OF
 UNLIMITED NOUTNM) (N=1,,5) (M=N+1), PARTICLES/SEC
 LSSNML = RATE OF LOSS OF PARTICLES, IN SIZE RANGE RN TO RM, FROM
 AEROSOL DUE TO SETTLING AND PLATEOUT (TIME DERIVATIVE OF
 LIMITED NOUTNM) (N=1,,5) (M=N+1), PARTICLES/SEC
 MASS = TOTAL MASS OF ALL THE PARTICLES REMAINING IN SUSPENSION
 AS AN AEROSOL IN THE CASK, GRAMS
 MINNM = NUMBER OF PARTICLES IN SIZE RANGE RN TO RM RELEASED TO THE
 AEROSOL FROM THE FUEL PINS IN THE X FUEL NODES (X=1,,5)
 (N=1,,5) (M=N+1), PARTICLES
 MNM = MASS OF A PARTICLE WITH RADIUS RNM (N=1,,5) (M=N+1),
 GRAMS/PARTICLE
 MTNM = TOTAL MASS OF PARTICLES IN THE SIZE RANGE RN TO RM
 RELEASED FROM ALL X FUEL NODES (SUM OF FREE AND BOUND-UP)
 (N=1,,5) (M=N+1) (X=1,,10), GRAMS
 MTUT = TOTAL MASS OF PARTICLES IN ALL SIZE RANGES RELEASED
 FROM ALL X FUEL NODES (SUM OF FREE AND BOUND-UP) (X=1,,5),
 GRAMS
 MTOTIN = KNOWN TOTAL MASS OF PARTICLES IN ALL OF NGRPS SIZE GROUPS
 NASSY = THE NUMBER OF FUEL ASSEMBLIES IN THE CASK
 NBNMX = NUMBER OF FREE PARTICLES IN THE SIZE RANGE RN TO RM
 RELEASED FROM FUEL NODE X WHEN FUEL PINS BURST (N=1,,5)
 (M=N+1) (X=1,,10), PARTICLES
 NGRPS = NUMBER OF PARTICLE SIZE GROUPS CONSIDERED.
 NNM = NUMBER OF PARTICLES IN SIZE RANGE RN TO RM REMAINING IN
 SUSPENSION AS AN AEROSOL IN THE CASK (N=1,,5) (M=N+1),
 PARTICLES
 NNMX = TOTAL NUMBER OF PARTICLES IN THE SIZE RANGE RN TO RM
 RELEASED FROM FUEL NODE X (SUM OF FREE AND ROUNDUP)
 (N=1,,5) (M=N+1) (X=1,,10), PARTICLES
 NONM = LOGICAL CONTROL VARIABLES (LCV), FUNCTION SWITCHES. TRUE
 OR ON IF NINNM.LE.NOUTNM, OFF OTHERWISE (N=1,,5) (M=N+1).

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
 for the IF-300 (Page 2 of 16)

. NOUTNM = NUMBER OF PARTICLES IN SIZE RANGE RN TO RM LOST FROM
 . AEROSOL DUE TO SETTLING AND PLATEOUT (N=1,,5)(M=N+1)
 . (RANGE OF NOUTNM LIMITED TO 0.LE.NOUTNM.LE.NINNM),
 . PARTICLES
 . NOXNMX = NUMBER OF BOUND-UP PARTICLES IN THE SIZE RANGE RN TO RM
 . RELEASED FROM FUEL NODE X WHEN THE EXPOSED FUEL IN FUEL
 . NODE X OXIDIZES TO U3O8 (N=1,,5)(M=N+1)(X=1,,10), PARTICLES
 . NPINS = THE NUMBER OF PINS PER SQ INCH OF FUEL ASSY, PINS/IN**2
 . NSCA = SCALE FACTOR FOR PLOT OF PARTICLE SIZE VS TIME.
 . NTNM = TOTAL NUMBER OF PARTICLES IN THE SIZE RANGE RN TO RM
 . RELEASED FROM ALL X FUEL NODES (SUM OF FREE AND BOUND-UP)
 . (N=1,,5)(M=N+1)(X=1,,10), PARTICLES
 . NTOT = TOTAL NUMBER OF PARTICLES IN ALL SIZE RANGES RELEASED
 . FROM ALL X FUEL NODES (SUM OF FREE AND BOUND-UP), PARTICLES
 . OSWJ = LOGICAL CONTROL VARIABLE (LCV), FUNCTION SWITCH. OSWJ=1.
 . WHEN TIME.GE.TOXJ, AND OSWJ=0. WHEN TIME.LT.TOXJ (J=1,,10)
 . OXIDATION SWITCH.
 . PHISX = VOLUME FRACTION OF PARTICLES RELEASED AS AN AEROSOL FROM
 . EACH OF X FUEL NODES (X=1,,10).
 . PNODEX = NUMBER OF FUEL PINS IN FUEL NODE X (X=1,,10), PINS/NODE
 . RFNM = PARTICLE RADIUS FACTOR FOR SIZE GROUP BOUNDED BY RN AND
 . RM (N=1,,5)(M=N+1), 1/CM**3
 . RHO = DENSITY OF PARTICLE, GM/CM**3
 . RMAX = MAX PARTICLE RADIUS, CM
 . RMIN = MIN PARTICLE RADIUS, CM
 . RN = RADII BOUNDING EACH PARTICLE SIZE GROUP (N=1,,6), CM
 . RNM = AVERAGE RADII OF PARTICLES IN SIZE GROUPS (N=1,,5)(M=N+1),
 . CM
 . SNOSEX = THE CROSS-SECTIONAL AREA OF FUEL ASSY PER FUEL NODE X
 . (IN THE HEAT TRANSFER CIRCUIT), IN**2 ASSY/NODE
 . SNOOP = NUMERICAL FLAG. ACTIVATES FUNCTION SWITCH CHCK WHEN
 . SNOOP.GT.0.
 . SUMENM = LOGICAL CONTROL VARIABLES (LCV), LOGICAL COMPLEMENTS OF
 . NONM. TRUE OR ON IF NINNM.GT.NOUTNM, OFF OTHERWISE
 . (N=1,,5)(M=N+1).
 . T = ELAPSED TIME OF SIMULATION, SECONDS
 . TBJ = THE TIME AT WHICH FUEL PINS BURST IN FUEL NODE J ((J=1,,10)
 . (OBTAINED FROM LOSS-OF-COOLANT MODEL), SECONDS
 . TEO = LOGICAL CONTROL VARIABLE (LCV), FUNCTION SWITCH. TRUE OR
 . ON IF (T+TLOCFB+DT).LE.TB1, OFF OTHERWISE.
 . TFIN = TIME LIMIT ON SIMULATION, SECONDS
 . TIME = T + TLOCFB, SECONDS
 . TLOCFB = START TIME BASED ON TIME REQUIRED FOR FIRST FUEL PINS TO
 . BURST IN THE LOSS-OF-COOLANT MODEL, SECONDS
 . TOXJ = THE TIME AT WHICH FUEL IN NODE J OXIDIZES TO U3O8 (J=1,,10)
 . (OBTAINED FROM LOSS-OF-COOLANT MODEL), SECONDS
 . VA = FREE VOLUME INSIDE CASK, IN**3
 . VCSK = FREE VOLUME INSIDE THE CASK, CM**3

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
 for the IF-300 (Page 3 of 16)

```

.      VG = VOLUME OF VOID SPACE IN FUEL NODE X (X=1,,10) , IN**3/NODE
.      VNM = VELOCITY OF FALL OF SETTLING PARTICLES RNM (N=1,,,5)
.           (M=N+1) , CM/SEC
.      VNX = TOTAL AEROSOL VOLUME IN FUEL NODE X (X=1,,10) , IN**3/NODE
.      VOID = VOLUME OF VOID SPACE IN EACH FUEL PIN, IN**3/PIN
.      VOLNM = VOLUME OF A PARTICLE WITH RADIUS RNM (N=1,,,5) (M=N+1) ,
.           CM**3/PARTICLE
.      VSOLPN = THE VOLUME OF VOLATILE SOLIDS PER PIN, IN**3/PIN
.      VSOLX = VOLUME OF VOLATILE SOLIDS IN FUEL NODE X (X=1,,10) ,
.           IN**3/NODE

```

INPUT

```

      PAR(RMAX,RMIN,NGRPS)
      PAR(TLOCLW)
      PAR(TFIN)
      PAR(TB1,TB2,TB3,TB7,TB8)
      PAR(TB9,TB10)
      PAR(TOX1,TOX2,TOX3,TOX7,TOX8)
      PAR(TOX9,TOX10)
      PAR(NSCA)
      PAR(SNOCP)
      PAR(RHO,G,FT4,VCSK)
      PAR(DC,DX,NPINS,FG,VSOLPN,VOID)
      PAR(SNODE1,SNODE2,SNODE3,SNODE7,SNODE8)
      PAR(SNODE9,SNODE0)
      PAR(CPM,FR,FSOL)
      PAR(OLDELT,ASURF)
      PAR(MTOTIN,FACT)

```

```

      USC      PFN(5.)
      DIFCOF = PFN(5.)

```

FUNCTION SWITCH TEO. TRUE OR ON IF (T+TLOCFB+DT).LE.TB1, OFF OTHERWISE.

```

      TEO      = FSW(T+TLOCFB+DT-TB1,TRUE,TRUE,FALSE)

```

RANGE OF RADII IN EACH PARTICLE SIZE GROUP

```

      TEO      DLTR      = (RMAX-RMIN)/NGRPS

```

RADII BOUNDING EACH SIZE GROUP

```

      TEO      R1        = RMIN
      TEO      R2        = R1+DLTR
      TEO      R3        = R2+DLTR
      TEO      R4        = R3+DLTR
      TEO      R5        = R4+DLTR
      TEO      R6        = R5+DLTR

```

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model for the IF-300 (Page 4 of 16)

AVERAGE RADII OF SIZE GROUPS

```

•
TEO      R12      = (1.5*(R2*R2-R1*R1)*(R1*R2))/(R2*R2*R2-R1*R1*R1)
TEO      R23      = (1.5*(R3*R3-R2*R2)*(R2*R3))/(R3*R3*R3-R2*R2*R2)
TEO      R34      = (1.5*(R4*R4-R3*R3)*(R3*R4))/(R4*R4*R4-R3*R3*R3)
TEO      R45      = (1.5*(R5*R5-R4*R4)*(R4*R5))/(R5*R5*R5-R4*R4*R4)
TEO      R56      = (1.5*(R6*R6-R5*R5)*(R5*R6))/(R6*R6*R6-R5*R5*R5)

```

CUNNINGHAM SLIP COEFFICIENTS

```

•
TEO      CSC12     FUN(CSC,R12)
TEO      CSC23     FUN(CSC,R23)
TEO      CSC34     FUN(CSC,R34)
TEO      CSC45     FUN(CSC,R45)
TEO      CSC56     FUN(CSC,R56)

```

VELOCITY OF FALL OF SETTLING PARTICLES

```

•
TEO      VLCTY     CSP(R12,CSC12)
TEO                               RSP(V12)
TEO      VLCTY     CSP(R23,CSC23)
TEO                               RSP(V23)
TEO      VLCTY     CSP(R34,CSC34)
TEO                               RSP(V34)
TEO      VLCTY     CSP(R45,CSC45)
TEO                               RSP(V45)
TEO      VLCTY     CSP(R56,CSC56)
TEO                               RSP(V56)

```

CALCULATION OF CASK SHAPE FACTOR FOR SETTLING TERMS

```

•
TEO      FCSK      (3.1416*(DC*DC-DX*DX))/(4.*VCSK)

```

CALCULATION OF SETTLING TERM COEFFICIENTS

```

•
TEO      C12       FCSK*V12
TEO      C23       FCSK*V23
TEO      C34       FCSK*V34
TEO      C45       FCSK*V45
TEO      C56       FCSK*V56

```

CONVERT VCSK (CM**3) TO VA (IN**3)

```

•
TEO      VA        .0610*VCSK

```

CALCULATION OF COMBINED SETTLING AND PLATEOUT LOSS COEFFICIENTS

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
for the IF-300 (Page 5 of 16)

•
CALCULATION OF PARTICLE RADIUS FACTOR

•
TEO RF12 = (R2-R1)/(R1*R1*R1*R1)
TEO RF23 = (R3-R2)/(R2*R2*R2*R2)
TEO RF34 = (R4-R3)/(R3*R3*R3*R3)
TEO RF45 = (R5-R4)/(R4*R4*R4*R4)
TEO RF56 = (R6-R5)/(R5*R5*R5*R5)

•
CALCULATION OF PLATEOUT DIFFUSION COEFFICIENTS

•
TEO DP12 = FUN(DIFCOF,R12)
TEO DP23 = FUN(DIFCOF,R23)
TEO DP34 = FUN(DIFCOF,R34)
TEO DP45 = FUN(DIFCOF,R45)
TEO DP56 = FUN(DIFCOF,R56)

•
CALCULATION OF SHAPE FACTOR FOR PLATEOUT TERMS

•
TEO DCOF = ASURF/(BLDELTA*VCSK)

•
CALCULATION OF PLATEOUT TERM COEFFICIENTS

•
TEO D12 = DCOF*DP12
TEO D23 = DCOF*DP23
TEO D34 = DCOF*DP34
TEO D45 = DCOF*DP45
TEO D56 = DCOF*DP56

•
COMBINED SETTLING AND PLATEOUT COEFFICIENTS

•
TEO CD12 = C12+D12
TEO CD23 = C23+D23
TEO CD34 = C34+D34
TEO CD45 = C45+D45
TEO CD56 = C56+D56

•
•
CALCULATION OF VOLUME FRACTION OF PARTICLES RELEASED AS AN AEROSOL FROM EACH FUEL NODE

•
TEO PHI CSP(SNODE1)
TEO RSP(FNODE1,VSOL1,VN1,PHIS1)
TEO PHI CSP(SNODE2)
TEO RSP(FNODE2,VSOL2,VN2,PHIS2)
TEO PHI CSP(SNODE3)
TEO RSP(FNODE3,VSOL3,VN3,PHIS3)
TEO PHI CSP(SNODE7)
TEO RSP(FNODE7,VSOL7,VN7,PHIS7)
TEO PHI CSP(SNODE6)
TEO RSP(FNODE6,VSOL6,VN6,PHIS6)
TEO PHI CSP(SNODE9)
TEO RSP(FNODE9,VSOL9,VN9,PHIS9)
TEO PHI CSP(SNODE0)
TEO RSP(FNODE0,VSOL0,VN0,PHIS0)

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
for the IF-300 (Page 6 of 16)

CALCULATION OF PARTICLE VOLUME, MASS, AND ACTIVITY

```

TEC      VMA      CSP (R1,R2)
TEC      RSP (VOL12,M12,ACT12)
TEC      VMA      CSP (R2,R3)
TEC      RSP (VOL23,M23,ACT23)
TEC      VMA      CSP (R3,R4)
TEC      RSP (VOL34,M34,ACT34)
TEC      VMA      CSP (R4,R5)
TEC      RSP (VOL45,M45,ACT45)
TEC      VMA      CSP (R5,R6)
TEC      RSP (VOL56,M56,ACT56)

```

CALCULATION OF NUMBER OF TOTAL, FREE, AND BOUND-UP PARTICLES AVAILABLE

```

TEC      NMBR      CSP (R1,R2,PHIS1,VN1,FACT)
TEC      RSP (N121,N3121,NOX121)
TEC      NMBR      CSP (R2,R3,PHIS1,VN1,FACT)
TEC      RSP (N231,N3231,NOX231)
TEC      NMBR      CSP (R3,R4,PHIS1,VN1,FACT)
TEC      RSP (N341,N3341,NOX341)
TEC      NMBR      CSP (R4,R5,PHIS1,VN1,FACT)
TEC      RSP (N451,N3451,NOX451)
TEC      NMBR      CSP (R5,R6,PHIS1,VN1,FACT)
TEC      RSP (N561,N3561,NOX561)
TEC      NMBR      CSP (R1,R2,PHIS2,VN2,FACT)
TEC      RSP (N122,N3122,NOX122)
TEC      NMBR      CSP (R2,R3,PHIS2,VN2,FACT)
TEC      RSP (N232,N3232,NOX232)
TEC      NMBR      CSP (R3,R4,PHIS2,VN2,FACT)
TEC      RSP (N342,N3342,NOX342)
TEC      NMBR      CSP (R4,R5,PHIS2,VN2,FACT)
TEC      RSP (N452,N3452,NOX452)
TEC      NMBR      CSP (R5,R6,PHIS2,VN2,FACT)
TEC      RSP (N562,N3562,NOX562)
TEC      NMBR      CSP (R1,R2,PHIS3,VN3,FACT)
TEC      RSP (N123,N3123,NOX123)
TEC      NMBR      CSP (R2,R3,PHIS3,VN3,FACT)
TEC      RSP (N233,N3233,NOX233)
TEC      NMBR      CSP (R3,R4,PHIS3,VN3,FACT)
TEC      RSP (N343,N3343,NOX343)
TEC      NMBR      CSP (R4,R5,PHIS3,VN3,FACT)
TEC      RSP (N453,N3453,NOX453)
TEC      NMBR      CSP (R5,R6,PHIS3,VN3,FACT)
TEC      RSP (N563,N3563,NOX563)
TEC      NMBR      CSP (R1,R2,PHIS7,VN7,FACT)

```

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model for the IF-300 (Page 7 of 16)

TEC		RSP(N127,N3127,NOX127)
TEC	NMBR	CSP(R2,R3,PHIS7,VN7,FACT)
TEC		RSP(N237,N3237,NOX237)
TEC	NMBR	CSP(R3,R4,PHIS7,VN7,FACT)
TEC		RSP(N347,N3347,NOX347)
TEC	NMBR	CSP(R4,R5,PHIS7,VN7,FACT)
TEC		RSP(N457,N3457,NOX457)
TEC	NMBR	CSP(R5,R6,PHIS7,VN7,FACT)
TEC		RSP(N567,N3567,NOX567)
TEC	NMBR	CSP(R1,R2,PHIS8,VN8,FACT)
TEC		RSP(N128,N3128,NOX128)
TEC	NMBR	CSP(R2,R3,PHIS8,VN8,FACT)
TEC		RSP(N238,N3238,NOX238)
TEC	NMBR	CSP(R3,R4,PHIS8,VN8,FACT)
TEC		RSP(N348,N3348,NOX348)
TEC	NMBR	CSP(R4,R5,PHIS8,VN8,FACT)
TEC		RSP(N458,N3458,NOX458)
TEC	NMBR	CSP(R5,R6,PHIS8,VN8,FACT)
TEC		RSP(N568,N3568,NOX568)
TEC	NMBR	CSP(R1,R2,PHIS9,VN9,FACT)
TEC		RSP(N129,N3129,NOX129)
TEC	NMBR	CSP(R2,R3,PHIS9,VN9,FACT)
TEC		RSP(N239,N3239,NOX239)
TEC	NMBR	CSP(R3,R4,PHIS9,VN9,FACT)
TEC		RSP(N349,N3349,NOX349)
TEC	NMBR	CSP(R4,R5,PHIS9,VN9,FACT)
TEC		RSP(N459,N3459,NOX459)
TEC	NMBR	CSP(R5,R6,PHIS9,VN9,FACT)
TEC		RSP(N569,N3569,NOX569)
TEC	NMBR	CSP(R1,R2,PHIS0,VN0,FACT)
TEC		RSP(N120,N3120,NOX120)
TEC	NMBR	CSP(R2,R3,PHIS0,VN0,FACT)
TEC		RSP(N230,N3230,NOX230)
TEC	NMBR	CSP(R3,R4,PHIS0,VN0,FACT)
TEC		RSP(N340,N3340,NOX340)
TEC	NMBR	CSP(R4,R5,PHIS0,VN0,FACT)
TEC		RSP(N450,N3450,NOX450)
TEC	NMBR	CSP(R5,R6,PHIS0,VN0,FACT)
TEC		RSP(N560,N3560,NOX560)

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
for the IF-300 (Page 8 of 16)

•
CALCULATION OF TOTAL PARTICLES, MASS, AND ACTIVITY

•
TEC NT12A ADD (N121,N122,N123,N127,N128)
TEC NT23A ADD (N231,N232,N233,N237,N238)
TEC NT34A ADD (N341,N342,N343,N347,N348)
TEC NT45A ADD (N451,N452,N453,N457,N458)
TEC NT56A ADD (N561,N562,N563,N567,N568)
TEC NT12 ADD (NT12A,N129,N120)
TEC NT23 ADD (NT23A,N239,N230)
TEC NT34 ADD (NT34A,N349,N340)
TEC NT45 ADD (NT45A,N459,N450)
TEC NT56 ADD (NT56A,N569,N560)
TEC MTCT ADD (NT12,NT23,NT34,NT45,NT56)
TEC MT12 M12*NT12
TEC MT23 = M23*NT23
TEC MT34 = M34*NT34
TEC MT45 M45*NT45
TEC MT56 M56*NT56
TEC MTCT ADD (MT12,MT23,MT34,MT45,MT56)

•
FUNCTION SWITCH ITERAT. TRUE OR ON IF ABS(MTOTIN-MTOT),GT.1., OFF OTHERWISE.

•
TEC ITERAT = FSW(ABS(MTOTIN-MTOT)-.0001,FALSE,FALSE,TRUE)

•
CALCULATION OF CORRECTION FACTOR FACT WHICH ADJUSTS THE DISTRIBUTION FUNCTION IN SUBPROGRAM NMBR TO GIVE THE CORRECT MASS AND ACTIVITY

•
ITERAT FACT = IMP(FACT,FACT*(1.+(MTOTIN-MTOT)/MTOTIN))

•
TEC AT12 ACT12*NT12
TEC AT23 ACT23*NT23
TEC AT34 ACT34*NT34
TEC AT45 ACT45*NT45
TEC AT56 ACT56*NT56
TEC ATOT ADD(AT12,AT23,AT34,AT45,AT56)

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
for the IF-300 (Page 9 of 16)

```

SUBPROGRAMS
.
SUBPROGRAM TO CALCULATE VELOCITY OF FALL
.
WHERE
.
.      V      = THE VELOCITY OF FALL, CM/SEC
.      RXY     = THE AVERAGE OF RADII RX AND RY, CM
.      CSCXY   = THE CUNNINGHAM SLIP COEFFICIENT FOR PARTICLE OF RADIUS RX
.
TEC      VLCTY   BSP(RXY,CSCXY)
TEC      V       (2.*RXY**RXY*RHO*G*CSCXY)/(9.*ETA)
TEC      VLCTY   ESP(V)
.
SUBPROGRAM TO CALCULATE VOLUME FRACTION OF PARTICLES IN AEROSOL
.
WHERE
.
.      PNODEX = THE NUMBER OF FUEL PINS IN NODE X, PINS/NODE
.      VSOLX  = THE VOLUME OF VOLATILE SOLIDS IN FUEL NODE X, IN**3/NODE
.              (IN THE VOID SPACE ONLY)
.      VG     = THE VOLUME OF VOID SPACE IN FUEL NODE X, IN**3/NODE
.      VOID   = THE VOLUME OF VOID SPACE IN EACH FUEL PIN, IN**3/PIN
.      VN     = THE TOTAL AEROSOL VOLUME IN NODE X, IN**3/NODE
.      PHISX  = THE FRACTION OF SOLIDS IN THE AEROSOL
.
TEC      PHI     BSP(SNODEX)
TEC      PNODEX  NPINS*SPNODEX
TEC      VSOLX   VSOLFN*PNODEX*FG
TEC      VG      PNODEX*VOID
TEC      VN      VG
TEC      PHISX   VSOLX/VN
TEC      PHI     ESP(PNODEX,VSOLX,VN,PHISX)
.
SUBPROGRAM TO CALCULATE NUMBER OF PARTICLES--TOTAL,FREE AND BOUND UP
.
WHERE
.
.      THE CONSTANT 16.387 CONVERTS VN FROM IN**3 TO CM**3
.      NT      = THE TOTAL NUMBER OF PARTICLES IN THE SIZE RANGE RA TO RB
.                PRESENT IN FUEL NODES OF MASSY FUEL ASSEMBLIES
.      NB      = THE NUMBER OF FREE PARTICLES IN NT WHICH ARE RELEASED WHE
.                THE PINS BURST
.      NOX     = THE NUMBER OF BOUND-UP PARTICLES IN NT RELEASED WHEN
.                FUEL IN NODEX OXIDIZES
.      THE FACTOR 0.679 ADJUSTS THE DISTRIBUTION FUNCTION TO GIVE THE
.      CORRECT MASS AND ACTIVITY. THE USE OF THIS FACTOR IS EQUIVALENT
.      TO REPLACING THE CONSTANT 0.05 BY .033.
.
TEC      NMBR     BSP(RA,RB,PHIS,VN,FCTR)
TEC      RA4      RA * RA * RA * RA
TEC      NT       (.05*(RB-RA)*PHIS*VN*16.387*FCTR) /RA4

```

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
for the IF-300 (Page 10 of 16)

```

      TEO      NB      FR * FSOL * NT
      TEO      NOX     FR * (1. - FSOL) * NT
      TEO      NMBR    ESP(NT,NB,NOX)
    .
SUBPROGRAM TO CALCULATE PARTICLE VOLUME,MASS,AND ACTIVITY
    .
WHERE
    .      RAB      = THE RADIUS OF A PARTICLE IN SIZE RANGE AB,CM/PARTICLE
    .      VAB      = THE VOLUME OF A PARTICLE WITH RADIUS RAB, CM**3/PARTICLE
    .      MAB      = THE MASS OF A PARTICLE WITH RADIUS RAB, GM/PARTICLE
    .      AAB      = THE ACTIVITY OF A PARTICLE OF RADIUS RAB,CURIES/PARTICLE
    .      RAA      = RA
    .      RBB      = RB
    .
      TEO      VMA      BSP(RAA,RBB)
      TEO      RA3      RAA* RAA* RAA
      TEO      RB3      RBB* RBB* RBB
      TEO      VAB      (4.*3.14*LOG(RBB/RAA))/((1./RA3)-(1./RB3))
      TEO      MAB      VAB*RHO
      TEO      AAB      CPM*MAB
      TEO      VMA      ESP(VAB,MAB,AAB)
    .
    .
CALCULATION OF TRANSIENT BEHAVIOR OF VOLATILE SOLIDS RELEASED AS AN
AEROSOL FROM FUEL PINS TO CONTAINMENT VESSEL AFTER PINS BURST
    .
    .
    .      (1) THIS MODEL BASED ON COAGULATION EQUATION FOR AEROSOLS HAVING A
    .          DISTRIBUTION OF PARTICLE SIZES, MODIFIED TO INCLUDE A SOURCE
    .          TERM AND TERMS FOR PARTICLE REMOVAL FROM THE AEROSOL BY SETTLIN
    .          AND PLATEOUT.
    .      (2) AGGLOMERATION TERMS ELIMINATED BY USING "SELF-PRESERVING)
    .          PARTICLE SIZE DISTRIBUTION FUNCTION.
    .
    .
    .
PARTICLE SOURCES (PARTICLES ADDED TO AEROSOL)      *****
    .
FUNCTION SWITCHES BSWJ (J=1,,,10) (BURST SWITCHES). BSWJ=1. WHEN
TIME.GE.TBJ AND BSWJ=0. WHEN TIME.LT.TBJ. TBJ IS THE TIME THE FUEL PI
BURST IN NODE J OF THE CASK LOSS-OF-COOLANT MODEL LOCFB.
    .
      BSW1      = FSW(TIME-TB1,0.,1.,1.)
      BSW2      = FSW(TIME-TB2,0.,1.,1.)
      BSW3      = FSW(TIME-TB3,0.,1.,1.)

```

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
for the IF-300 (Page 11 of 16)

```

BSW7   = FSW (TIME-TB7,0.,1.,1.)
BSW8   = FSW (TIME-TB8,0.,1.,1.)
BSW9   = FSW (TIME-TB9,0.,1.,1.)
BSW10  = FSW (TIME-TB10,0.,1.,1.)

```

FUNCTION SWITCHES OSWJ (J=1,,10) (OXIDATION SWITCHES). OSWJ=1. WHEN TIME.GE.TOXJ AND OSWJ=0. WHEN TIME.LT.TOXJ. TOXJ IS THE TIME THE EXPOSED FUEL OXIDIZES IN THE FUEL PINS WHICH HAVE BURST IN NODE J OF CASK LOSS-OF-COOLANT MODEL LUCFB.

```

OSW1   = FSW (TIME-TOX1,0.,1.,1.)
OSW2   = FSW (TIME-TOX2,0.,1.,1.)
OSW3   = FSW (TIME-TOX3,0.,1.,1.)
OSW7   = FSW (TIME-TOX7,0.,1.,1.)
OSW8   = FSW (TIME-TOX8,0.,1.,1.)
OSW9   = FSW (TIME-TOX9,0.,1.,1.)
OSW10  = FSW (TIME-TOX10,0.,1.,1.)

```

CALCULATION OF NUMBER OF PARTICLES IN EACH SIZE RANGE RELEASED (FROM FUEL PINS IN VARIOUS FUEL NODES) TO THE AEROSOL.

```

N12A   = BSW1*N121+BSW2*N122+BSW3*N123+BSW7*N127
N12B   = N12A+BSW8*N128+BSW9*N129+BSW10*N120
N12C   = N12B+OSW1*NOX121+OSW2*NOX122+OSW3*NOX123
N12D   = N12C+OSW7*NOX127+OSW8*NOX128+OSW9*NOX129
NIN12  = N12D+OSW10*NOX120
N23A   = BSW1*N231+BSW2*N232+BSW3*N233+BSW7*N237
N23B   = N23A+BSW8*N238+BSW9*N239+BSW10*N230
N23C   = N23B+OSW1*NOX231+OSW2*NOX232+OSW3*NOX233
N23D   = N23C+OSW7*NOX237+OSW8*NOX238+OSW9*NOX239
NIN23  = N23D+OSW10*NOX230
N34A   = BSW1*N341+BSW2*N342+BSW3*N343+BSW7*N347
N34B   = N34A+BSW8*N348+BSW9*N349+BSW10*N340
N34C   = N34B+OSW1*NOX341+OSW2*NOX342+OSW3*NOX343
N34D   = N34C+OSW7*NOX347+OSW8*NOX348+OSW9*NOX349
NIN34  = N34D+OSW10*NOX340
N45A   = BSW1*N451+BSW2*N452+BSW3*N453+BSW7*N457
N45B   = N45A+BSW8*N458+BSW9*N459+BSW10*N450
N45C   = N45B+OSW1*NOX451+OSW2*NOX452+OSW3*NOX453
N45D   = N45C+OSW7*NOX457+OSW8*NOX458+OSW9*NOX459
NIN45  = N45D+OSW10*NOX450
N56A   = BSW1*N561+BSW2*N562+BSW3*N563+BSW7*N567
N56B   = N56A+BSW8*N568+BSW9*N569+BSW10*N560
N56C   = N56B+OSW1*NOX561+OSW2*NOX562+OSW3*NOX563
N56D   = N56C+OSW7*NOX567+OSW8*NOX568+OSW9*NOX569
NIN56  = N56D+OSW10*NOX560

```

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model for the IF-300 (Page 12 of 16)

REMOVAL OR LOSS OF PARTICLES FROM AEROSOL *****

RATE OF LOSS OF PARTICLES FROM AEROSOL DUE TO SETTLING AND PLATEOUT.

```

TE0      A12      = CD12*.05*RF12
TE0      A23      = CD23*.05*RF23
TE0      A34      = CD34*.05*RF34
TE0      A45      = CD45*.05*RF45
TE0      A56      = CD56*.05*RF56
TE0      3R12     = PWR(R12,3.)
TE0      3R23     = PWR(R23,3.)
TE0      3R34     = PWR(R34,3.)
TE0      3R45     = PWR(R45,3.)
TE0      3R56     = PWR(R56,3.)
TE0      COF      = 4.*3.14/3.

DISTA    = 3R12*N12+3R23*N23+3R34*N34+3R45*N45+3R56*N56
DIST     = COF*DISTA
LOSS12   = A12*DIST
LOSS23   = A23*DIST
LOSS34   = A34*DIST
LOSS45   = A45*DIST
LOSS56   = A56*DIST

```

CALCULATION OF NUMBER OF PARTICLES IN EACH SIZE RANGE LOST FROM THE AEROSOL DUE TO SETTLING AND PLATEOUT.

```

LSS12L = LIN(LOSS12,NOUT12,0.,NIN12)
NOUT12 = INT(LSS12L,0.)
LSS23L = LIN(LOSS23,NOUT23,0.,NIN23)
NOUT23 = INT(LSS23L,0.)
LSS34L = LIN(LOSS34,NOUT34,0.,NIN34)
NOUT34 = INT(LSS34L,0.)
LSS45L = LIN(LOSS45,NOUT45,0.,NIN45)
NOUT45 = INT(LSS45L,0.)
LSS56L = LIN(LOSS56,NOUT56,0.,NIN56)
NOUT56 = INT(LSS56L,0.)

```

PARTICLES REMAINING IN SUSPENSION AS AN AEROSOL *****

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model for the IF-300 (Page 13 of 16)

•
 FUNCTION SWITCHES NONM (N=1,,5) (M=N+1). TRUE OR ON IF NINNM.LE.NOUTNM,
 OFF OTHERWISE. THIS LCV ASSURES A NON-NEGATIVE VALUE FOR THE NUMBER OF
 PARTICLES REMAINING IN SUSPENSION.

•
 N012 = FSW(NIN12-NOUT12,TRUE,TRUE,FALSE)
 N023 = FSW(NIN23-NOUT23,TRUE,TRUE,FALSE)
 N034 = FSW(NIN34-NOUT34,TRUE,TRUE,FALSE)
 N045 = FSW(NIN45-NOUT45,TRUE,TRUE,FALSE)
 N056 = FSW(NIN56-NOUT56,TRUE,TRUE,FALSE)

•
 LOGICAL CONTROL VARIABLES (LCV) SOMENM, THE LOGICAL COMPLEMENTS OF NONM
 (N=1,,5) (M=N+1).

•
 SOME12 = NOT(N012)
 SOME23 = NOT(N023)
 SOME34 = NOT(N034)
 SOME45 = NOT(N045)
 SOME56 = NOT(N056)

•
 CALCULATION OF NUMBER OF PARTICLES REMAINING IN SUSPENSION AS AN AEROSOL

•
 N012 N12 = 0.
 N023 N23 = 0.
 N034 N34 = 0.
 N045 N45 = 0.
 N056 N56 = 0.
 SOME12 N12 = NIN12-NOUT12
 SOME23 N23 = NIN23-NOUT23
 SOME34 N34 = NIN34-NOUT34
 SOME45 N45 = NIN45-NOUT45
 SOME56 N56 = NIN56-NOUT56

•
 CALCULATION OF TOTAL ACTIVITY OF PARTICLES IN AEROSOL

•
 ACTVTY = ACT12*N12+ACT23*N23+ACT34*N34+ACT45*N45+ACT56*N56
 ACTOA = ACT12*NOUT12+ACT23*NOUT23+ACT34*NOUT34+ACT45*NOUT45
 ACTOUT = ACTOA+ACT56*NOUT56
 ACTBAL = ACTVTY+ACTOUT

•
 CALCULATION OF TOTAL MASS OF PARTICLES IN AEROSOL

•
 MASS = M12*N12+M23*N23+M34*N34+M45*N45+M56*N56

•
 COMPUTE TIME IN SECONDS AND HOURS

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
 for the IF-300 (Page 14 of 16)


```

      TIME   = T+TLOGCLW
      HOURS  = TIME/3600.
.
STOP COMPUTATIONS WHEN TIME = TFIN
.
      FIN(TIME,TFIN)
.
FUNCTION SWITCH CHCK.  TRUE OR ON WHEN SNOOP.GT.0., OFF OTHERWISE.  USED
FOR PRINTING SELECTED OUTPUT FOR CHECK PURPOSES.
.
      CHCK   = FSW(SNOOP,FALSE,FALSE,TRUE)
.
TIME STEP FOR PRINTOUT
.
      DT     = 60.
.
OUTPUT
.
      OUT(TIME,N12,N23,N34,N45,N56)
      OUT(HOURS,NIN12,NIN23,NIN34,NIN45,NIN56)
      OUT( ,NOUT12,NOUT23,NOUT34,NOUT45,NOUT56)
      OUT( ,LSS12L,LSS23L,LSS34L,LSS45L,LSS56L)
      OUT( ,LOSS12,LOSS23,LOSS34,LOSS45,LOSS56)
      OUT( ,ACTVTY,MASS,ACTOUT,ACTBAL)
      OUT( ,MTOT,MTOTIN,FACT,ATOT)
      OUT( ,R1,R2,R3,R4,R5)
      OUT( ,R6,R12,R23,R34,R45)
      OUT( ,R56)
      OUT( ,3R12,3R23,3R34,3R45,3R56)
      OUT( ,DLTH,FOSK,VA,VOSK)
      OUT( ,PHIS1,PHIS2,PHIS3,PHIS7,PHIS8)
      OUT( ,PHIS9,PHIS0)
      OUT( ,VN1,VN2,VN3,VN7,VN8)
      OUT( ,VN9,VN0)
      OUT( ,C12,C23,C34,C45,C56)
      OUT( ,CSC12,CSC23,CSC34,CSC45,CSC56)
      OUT( ,D12,D23,D34,D45,D56)
      OUT( ,DP12,DP23,DP34,DP45,DP56)
      OUT( ,V12,V23,V34,V45,V56)
      OUT( ,N121,N3121,NOX121)
      OUT( ,N231,N3231,NOX231)
      OUT( ,N341,N341,NOX341)
      OUT( ,N451,N3451,NOX451)
      OUT( ,N561,N3561,NOX561)
      OUT( ,N122,N3122,NOX122)
      OUT( ,N232,N3232,NOX232)
      OUT( ,N342,N342,NOX342)
      OUT( ,N452,N3452,NOX452)
      OUT( ,N562,N3562,NOX562)

```

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model
for the IF-300 (Page 15 of 16)

```

TEO      OUT( ,N123,NB123,NOX123)
TEC      OUT( ,N233,NB233,NOX233)
TEO      OUT( ,N343,NB343,NOX343)
TEO      OUT( ,N453,NB453,NOX453)
TEC      OUT( ,N563,NB563,NOX563)
TEO      OUT( ,N127,NB127,NOX127)
TEC      OUT( ,N237,NB237,NOX237)
TEO      OUT( ,N347,NB347,NOX347)
TEO      OUT( ,N457,NB457,NOX457)
TEC      OUT( ,N567,NB567,NOX567)
TEO      OUT( ,N128,NB128,NOX128)
TEO      OUT( ,N238,NB238,NOX238)
TEC      OUT( ,N348,NB348,NOX348)
TEC      OUT( ,N458,NB458,NOX458)
TEC      OUT( ,N568,NB568,NOX568)
TEO      OUT( ,N129,NB129,NOX129)
TEO      OUT( ,N239,NB239,NOX239)
TEC      OUT( ,N349,NB349,NOX349)
TEO      OUT( ,N459,NB459,NOX459)
TEC      OUT( ,N569,NB569,NOX569)
TEO      OUT( ,N120,NB120,NOX120)
TEC      OUT( ,N230,NB230,NOX230)
TEO      OUT( ,N340,NB340,NOX340)
TEC      OUT( ,N450,NB450,NOX450)
TEO      OUT( ,N560,NB560,NOX560)
TEC      OUT( ,VOL12,M12,ACT12)
TEO      OUT( ,VOL23,M23,ACT23)
TEC      OUT( ,VOL34,M34,ACT34)
TEO      OUT( ,VOL45,M45,ACT45)
TEC      OUT( ,VOL56,M56,ACT56)
CHCK     OUT( ,BSW1,BSW2,BSW3,BSW7,BSW8)
CHCK     OUT( ,BSW9,BSW10)
CHCK     OUT( ,OSW1,OSW2,OSW3,OSW7,OSW8)
CHCK     OUT( ,OSW9,OSW10)
          OUT
          OUT
          PLO(HOURS,N12,N23,N34,N45,N56)
          SCA(.2,NSCA,NSCA,NSCA,NSCA,NSCA)
          ZER(0.,0.,0.,0.,0.,0.)
          TTP(VOL SOLIDS PARTICLE CONCENTRATIONS)
          TTY(NUMBER OF PARTICLES IN EACH SIZE GRP)
          TTX(TIME IN HOURS)
          PLO(HOURS,ACTVITY)
          SCA(0.2,2.)
          ZER(0.,0.)
          TTP(VOLATILE SOLIDS ACTIVITY)
          TTY(VOLATILE SOLIDS ACTIVITY, CURIES)
          TTX(TIME IN HOURS)
          END

```

FIGURE 4-2. MIMIC Listing of the Volatile Solids Release Model for the IF-300 (Page 16 of 16)

$A_-(v,t)$ = the rate at which particles of volume v are lost by agglomeration to yield larger particles, particles/cm³ (aerosol) x sec.

$R(v,t)$ = the rate at which particles of volume v are removed from the system by settling (fallout), leakage from the cask, and by deposition (plateout) on the walls of the containment vessel and any other "cold" surfaces in the cask, particles/cm³ (aerosol) x sec, and

$S(v,t)$ = the aerosol production rate, i.e., the rate at which particles of volume v are added to the system upon bursting of the fuel pins, particles/cm³ (aerosol) x sec.

In this study, this equation was further modified by eliminating the agglomeration terms by using the "self-preserving" particle size distribution function.

The agglomeration term A_+ represents a rate of formation (addition) of particles to the size group by coagulation of particles of smaller size, and the term A_- represents a rate of loss of particles from the size group due to coagulation to form particles of larger size (and transfer to a size group containing larger particles) (see Figure 4-5). If one assumes that these "transfers" of particles between particle size groups occur at rates that maintain a particular particle size distribution throughout the life of the aerosol, and that this distribution holds for any quantities of aerosol added to or taken away from the main aerosol, such as by pin bursting, settling, plateout, etc., then the "transfer terms" may be eliminated by using the assumed particular particle size distribution function to define the particle size distribution in these various source and removal terms. This is based on an approach suggested by Davis on pp. 36-46 of ORNL-4437 (Reference 13). In the present model, the "self-preserving" particle size distribution function was assumed. In this distribution function there is a term ϕ defined as the volume fraction of particles dispersed in

the aerosol, i.e., the ratio of the volume of all particles suspended in the aerosol to the total volume of the aerosol. When the particles of a particular size range are being considered and the particle balance equation is being evaluated for this particular size range, the transfer terms are dropped and the number of particles in this range, in the remaining source and removal terms, is expressed in terms of the "self-preserving" particle size distribution. The numbers of particles in all the other size ranges in the aerosol are related to the number of particles in the size range being considered through the volume fraction ϕ in the source and removal terms. Before it can be shown how this is done, the particle size distribution function must be discussed, the settling and plateout terms must be derived, and the source term must be derived for the pulsed inputs representing the release of free and bound up mixtures of fission gases and volatile solids from the bursting fuel pins. The self-preserving particle size distribution function used was obtained from the work of Davis.⁽¹³⁾ The settling and plateout terms were also first derived by Davis. These derivations are repeated here using a slightly different approach in each case.

4.1.1 Particle Size Distribution Function

According to Davis,⁽¹³⁾ the concept of the "self-preserving" size distribution has both theoretical and experimental basis. He points out that the concept is a steady-state size distribution resulting from coagulation (a process that makes big particles from little ones) and settling (which preferentially removes big particles). He also states that "The self-preserving distribution may well describe aerosols in a containment; in fact, it is not unlikely that the self-preserving distribution is achieved with highly coagulated aerosols soon after nucleation."

The self-preserving distribution function is

$$\frac{dn(v,t)}{dr} = 0.05 \phi r^{-4} \quad (4-2)$$

where

ϕ = the volume fraction of disperse phase, cm^3 of particles/ cm^3 of aerosol, and

r = the radius of a particle of volume v , cm.

In order for Equation (4-2) to be dimensionally correct, the coefficient 0.05 must be in units of particles. Before it can be shown how the "self-preserving" distribution function can be used to eliminate the agglomeration terms in the coagulation equation, Equation (4-1), the removal and source terms in this equation must be derived.

4.1.2 Rate of Particle Removal from the Aerosol

The removal term, $R(v,t)$, in Equation (4-1) includes removal of particles from the system by settling, leakage and plateout. At the present stage of model development, only settling and plateout have been included. However, since the present model was completed, a leakage term representing the loss of particles through the breach in the cask containment has been developed and will be included in the model during the next development phase. The general concept of the leakage term is presented in Section 4.1.5, along with a discussion of the modifications required to include it in the present model.

4.1.2.1 Particle Removal by Settling

The particle settling term is based on the concept that the aerosol in the cask is well-stirred, i.e., that the concentration of particles in each of the size groups considered is the same everywhere in the free volume in the cask, except in the boundary layer between the cask volume and the available floor space. There is no mixing in the boundary layer. The particle settling term is also based on the assumption that all the particles obey Stoke's law, and that the velocity at which the particles fall through the boundary layer to the floor may be determined from this law.

Consider a particle balance on a size group containing particles with an average radius of r_{ij} , with no source of particles and with the only loss of particles due to stirred settling:

$$\left[\begin{array}{c} \text{Rate of change of} \\ \text{number of particles} \\ \text{in the size group} \end{array} \right] = \left[\begin{array}{c} \text{Input} \\ \text{Rate} \end{array} \right] - \left[\begin{array}{c} \text{Output} \\ \text{Rate} \end{array} \right] \quad (4-3)$$

or

$$\frac{dn_{ij}}{dt} = 0 - R_{Sij} \quad (4-4)$$

where

V_{CSK} = the free volume inside the cask, and the volume of the aerosol containing all size groups, cm^3 ,

n_{ij} = the number of particles with an average radius of r_{ij} (ranging from r_i to r_j) present in the cask, particles/ cm^3 of aerosol,

R_{Sij} = the rate at which particles with an average radius of r_{ij} are removed from the aerosol by settling, particles/ cm^3 aerosol x sec.

The rate at which the particles of average radius r_{ij} pass through the boundary layer on the floor and fall to the floor is

$$R_{Sij} = \frac{n_{ij} v_{fij} A_f}{V_{CSK}} \quad (4-5)$$

where

$V_{f\ ij}$ = the velocity of fall of a particle of radius r_{ij} through the aerosol in the cask (and through the boundary layer on the floor), cm/sec,

A_f = the surface area of the floor, cm^2 .

Therefore, the particle balance equation [Equation (4-4)] may be written as

$$\frac{dn_{ij}}{dt} = \frac{-n_{ij} V_{f\ ij} A_f}{V_{\text{CSK}}} . \quad (4-6)$$

The settling velocity or velocity of fall, $V_{f\ ij}$, is determined from Stoke's law. Stoke's law is simply a force balance on a particle falling at a constant velocity through some medium. Assuming the particle to be spherical, the force balance is derived as follows. A spherical particle of mass m_{ij} falling vertically through the medium is subjected to two forces, a viscous drag force and the force of gravity. A sketch of this sphere and the forces acting is shown below:

A force balance on this sphere may be written as

$$\Sigma F = m_{ij} a_{ij} \quad (4-7)$$

or

$$F_d - F_g = m_{ij} \frac{dv_{f_{ij}}}{dt} \quad (4-8)$$

where

$$\begin{aligned} F_d &= \text{the viscous drag force, } F \\ F_g &= \text{the force of gravity on the particle, } F \\ m_{ij} &= \text{the mass of the particle, } M \\ v_{f_{ij}} &= \text{the velocity of fall of the particle } \frac{L}{\theta} . \end{aligned}$$

The force on the particle due to gravity is

$$F_g = m_{ij}g \quad (4-9)$$

where

$$g = \text{the acceleration of gravity, } L/\theta^2 .$$

The frictional force of viscous drag for a spherical body of radius r_{ij} , moving at a velocity $v_{f_{ij}}$ in a continuous medium, is

$$F_d = 6\pi\eta r_{ij} v_{f_{ij}} \quad (4-10)$$

where

$$\eta = \text{the viscosity of the medium, } F/L^2\theta .$$

Substituting from Equations (4-9) and (4-10) into the force balance Equation (4-8) we get

$$6\pi\eta r_{ij} v_{f_{ij}} - m_{ij}g = m_{ij} \frac{dv_{f_{ij}}}{dt} , \quad (4-11)$$

but since the body is assumed to be moving through the medium at a constant velocity of $v_{f_{ij}}$, the inertial term is zero, and Equation (4-11) becomes

$$6\pi\eta r_{ij} v_{f_{ij}} = m_{ij}g . \quad (4-12)$$

Solving for the velocity of fall, Equation (4-12) becomes

$$v_{f_{ij}} = \frac{m_{ij}g}{6\pi\eta r_{ij}} . \quad (4-13)$$

The mass of the spherical particle is

$$m_{ij} = \frac{4}{3} \pi r_{ij}^3 \rho , \quad (4-14)$$

where

ρ = the density of the particle, M/L^3 .

Substituting the mass of Equation (4-14) into Equation (4-13), the velocity of fall becomes

$$v_{f_{ij}} = \frac{2 r_{ij}^2 \rho g}{9\eta} . \quad (4-15)$$

When the particle diameter is on the order of or smaller than the mean free path of molecules in the medium, the assumption of a continuous medium (continuum) is no longer valid. The drag on the particle is now mainly due to collisions with the molecules, and the particle falls freely, or slips, between collisions. Under these conditions, Equation (4-15) is no longer applicable. However, a correction factor applied to Stoke's law restores the validity of this equation. The correction factor is called the Cunningham slip coefficient, C . Applying this factor to Equation (4-15), the velocity of fall is

$$v_{f_{ij}} = \frac{2 r_{ij}^2 \rho g C}{9\eta} . \quad (4-16)$$

The Cunningham slip coefficient as a function of particle diameter is presented as Figure 4-3.⁽¹³⁾

FIGURE 4-3. Cunningham Coefficient at Room Conditions (Reference 13)

In the AMCO cask, the area upon which the particles settle, the floor area A_f , is assumed to be that area between the volume expansion chamber wall and the inside surface of the canister,

$$A_f = \frac{\pi}{4} (D_C^2 - D_X^2) \quad (4-17)$$

where

D_C = the inside diameter of the canister, cm

D_X = the outside diameter of the volume expansion chamber, cm.

For the IF-300, $D_X = 0$, and D_C would be the inside diameter of the cavity.

4.1.2.2 Particle Removal by Plateout

The term for particle removal from an aerosol due to plating out on colder surfaces bounding the aerosol is based on the concept that the particles diffuse through the boundary layer at the surfaces. It is assumed that the aerosol in the cask is well stirred so that the concentration is the same everywhere except in the boundary layer. According to Davis,⁽¹³⁾ a poorly stirred aerosol is not only difficult to model but, physically, reduces plateout substantially.

Consider a particle balance on a size group containing particles with an average radius of r_{ij} , with no source of particles and with the only loss of particles due to plateout on a surface bounding a well stirred aerosol:

$$\left[\begin{array}{l} \text{Rate of change of} \\ \text{number of particles} \\ \text{in size group} \end{array} \right] = \left[\begin{array}{l} \text{Input} \\ \text{Rate} \end{array} \right] - \left[\begin{array}{l} \text{Output} \\ \text{Rate} \end{array} \right] \quad (4-18)$$

or

$$\frac{dn_{ij}}{dt} = 0 - R_{p_{ij}} \quad (4-19)$$

where

$R_{p_{ij}}$ = the rate at which particles with an average radius or r_{ij} are removed from the aerosol by plating out on the bounding colder surfaces, particles/cm³ aerosol x sec.

Since plateout is based on the concept that the particles diffuse through the boundary layer at the surfaces, Equation (4-19) is written as

$$-\frac{dn_{ij}}{dt} = \frac{D_{p_{ij}} A_{SURF}}{\delta V_{CSK}} (n_{ij} - 0) = R_{p_{ij}} \quad (4-20)$$

where

A_{SURF} = the surface area of the bounding colder surfaces, cm²,

V_{CSK} = the free volume in the cask (assumed to be the volume of the aerosol in the cask), cm³ aerosol in cask,

$D_{p_{ij}}$ = the coefficient for diffusion of particles of radius r_{ij} through the boundary layer, cm²/sec,

δ = the boundary layer thickness, cm,

n_{ij} = the concentration or number of particles at the cask containment side of the boundary layer, particles/cm³ aerosol in cask. (The number of particles at the surface is zero because the particles become part of the surface and no longer exist as particles in the aerosol.)

The diffusion coefficient varies substantially with particle size as shown in Figure 4-4.⁽¹³⁾

FIGURE 4-4. Diffusion Coefficient of Particles (Reference 13)

Considerable uncertainty is introduced into Equation (4-20) due to the uncertainty of any estimation of the boundary layer thickness. Following the lead of Davis,⁽¹³⁾ a value of 0.1 cm was assumed for δ . Davis points out, however, that this value is probably in the low end of the range of possible values and would yield a high plateout rate estimate. He cites a reference in which the estimation of δ is discussed, but points out that the estimation is uncertain. This is analogous to the dilemma faced by investigators studying heat transfer by convection from a fluid to a bounding surface. Some, if not most, of these investigators visualize the heat transfer to the surface as a conduction mechanism that could be represented by an equation similar to Equation (4-20):

$$- \rho CV \frac{dT}{dt} = \frac{kA_{\text{SURF}}}{\delta} (T - T_s) \quad (4-21)$$

where

ρCV = the thermal capacity of the fluid, H/T,

T = the temperature of the fluid, T,

T_s = the temperature of the bounding surface, T,

k = the thermal conductivity of the fluid in the boundary layer, H/θLT.

Because of the difficulty in estimating the value of δ , and the uncertainty of any such estimation, a film or convective coefficient was defined as

$$h = \frac{k}{\delta} \quad (4-22)$$

which is determined experimentally. Before the removal of particles from an aerosol by plateout can be determined with any reasonable accuracy, perhaps a similar film coefficient will have to be determined experimentally.

The particle balance equation [Equation (4-20)] may be rewritten as

$$\frac{dn_{ij}}{dt} = \frac{-D_{pij} A_{\text{SURF}} n_{ij}}{\delta V_{\text{CSK}}} \quad (4-23)$$

4.1.3 Rate of Aerosol Production

The aerosol production rate term or particle source term of Equation (4-1) represents the releases of aerosol from the fuel pins when they burst, and again if the exposed fuel oxidizes to U_3O_8 . When the fuel pins first burst, the aerosol released consists of "free" fission gases and volatile solids or solid fission products (cesium compounds). Later, if the exposed fuel in the burst pins oxidize to U_3O_8 , the remaining "bound up" fission gases and volatile solids are released as an aerosol.

The released quantities of aerosol contain particles of solids in several sizes, ranging from those with a minimum radius of $r_{\min}$ to a maximum radius of $r_{\max}$. The number of particles is assumed to be distributed among N_{GPS} size groups, according to the "self-preserving" particle size distribution function of Equation (4-2).

Seven nodes are used to represent radial increments of the fuel assemblies in the loss-of-coolant model of the IF-300 (see Figures 3-19 and 3-20). As the temperature distributions in the fuel assemblies develop with time following the loss of coolant, each of these fuel nodes will be at different temperatures. Some will reach the temperature at which the fuel pins burst before others and, if oxidation is possible, some will reach the oxidation point before others. This means that the release of aerosol from the fuel pins in the seven fuel nodes may occur at different times. It is assumed that the releases are instantaneous, that is, there is no distinguishable rate of release, but rather that the release of particles are pulsed releases which may be represented by impulse functions.

Consider a particle balance on a size group containing particles with an average radius of r_{ij} which receives particles from a source, but which does not lose any particles.

The particle balance is

$$\frac{dn_{ij}}{dt} = S_{ij} \quad (4-24)$$

where

S_{ij} = the rate at which particles with an average radius of r_{ij} are added to the size group, particles/cm³ aerosol in cask x sec.

In terms of an impulse function and the number of particles added to the aerosol in the cask, Equation (4-24) becomes

$$\frac{dn_{ij}}{dt} = n_{S_{ij}} \delta(t) \frac{V_N}{V_{CSK}} \quad (4-25)$$

where

$n_{S_{ij}}$ = the number of particles contributed by the source, particles/cm³ aerosol in the source. [Note that the number of particles from the source is denoted by $n_{S_{ij}}$ rather than n_{ij} . This is because $n_{S_{ij}}$ is expressed as the number of particles in a cm³ of aerosol in the source whereas n_{ij} is expressed as the number of particles in a cm³ of aerosol in the cask.]

$\delta(t)$ = the Dirac impulse function, 1/sec

= 0 when $t < t_B$

= 1 when $t = t_B$

= 0 when $t > t_B$

t_B = the time at which the particles are released from the source, sec,

V_N = the volume of aerosol in the source which is released to the cask, cm³ aerosol in the source,

V_{CSK} = the volume of the aerosol in the cask (assumed to be the free volume in the cask), cm^3 aerosol in the cask or cm^3 of cask volume.

The total number of particles contributed by the source is

$$\int_0^{n_{ij}} dn_{ij} = n_{S_{ij}} \frac{V_N}{V_{CSK}} \int_0^t \delta(t) dt \quad (4-26)$$

or

$$n_{ij} = n_{S_{ij}} \frac{V_N}{V_{CASK}} H(t) \quad (4-27)$$

where

$$\begin{aligned} H(t) &= \text{Heaviside's unit function} \\ &= 0 \text{ when } t < t_B \\ &= 1 \text{ when } t \geq t_B, \end{aligned}$$

and $n_{ij} = 0$ at $t = 0$.

If there were n_{ijo} particles in the size group before the contribution from the source, then the number of particles in the size group would be

$$n_{ij} = n_{ijo} + n_{S_{ij}} \frac{V_N}{V_{CSK}} H(t) \quad (4-28)$$

where

n_{ijo} = the initial value of n_{ij} .

The unit function $H(t)$ is represented in the simulation model by the fuel pin clad burst switches BSW_k and the fuel oxidation switches OSW_k , where k denotes the k -th fuel node.

4.1.4 Modification of the Particle Balance Equation to Eliminate the Agglomeration Terms

It was stated at the beginning of this section that the agglomeration or particle transfer terms in the general particle balance equation, Equation

(4-1), could be eliminated if it is assumed that these rates are such that they maintain a particular particle size distribution throughout the life of the aerosol, provided that the same particle size distribution holds for any quantities of aerosol added to or removed from the main aerosol. A "self-preserving" particle size distribution function was chosen to represent the distribution of particles throughout the life of the aerosol. This distribution has been presented and discussed in Section 4.1.1. Terms have been derived in Section 4.1.2 that represent the rate of particle removal from the aerosol by settling and by plating out of particles on the colder surfaces bounding the aerosol. Also, a term representing the rate of aerosol production (a source term) has been derived in Section 4.1.3. It will now be shown how these terms and the self-preserving particle size distribution function can be combined to eliminate the need for the agglomeration terms that represent the rate of transfer of particles from one size group to another (see Figure 4-5).

The aerosol is arbitrarily divided into several size groups, and a particle balance equation, without agglomeration terms, is written for each of these size groups. The numbers of particles in the source and removal terms are expressed in terms of the self-preserving particle size distribution function. The numbers of particles in all the other size groups are related to the number of particles in the size group considered through the volume fraction ϕ in the particle size distribution function.

Five particle size groups were considered, encompassing particles from a minimum radius $r_{\min}$ to a maximum radius $r_{\max}$. A size range increment for this spread of particle sizes was determined by dividing the range by the number of size groups

$$\Delta r = \frac{r_{\max} - r_{\min}}{N_{\text{GPS}}} \quad (4-29)$$

where

Δr = the particle radius increment for each size group, L,

$r_{\max}$ = the maximum particle radius considered, L,

$r_{\min}$ = the minimum particle radius considered, L,

N_{GPS} = the desired number of particle size groups to be considered.

The radii bounding each of the five size groups considered are:

$$r_1 = r_{\min} \quad (4-30)$$

$$r_2 = r_1 + \Delta r \quad (4-31)$$

$$r_3 = r_2 + \Delta r \quad (4-32)$$

$$r_4 = r_3 + \Delta r \quad (4-33)$$

$$r_5 = r_4 + \Delta r \quad (4-34)$$

and
$$r_6 = r_5 + \Delta r = r_{\max} . \quad (4-35)$$

The weighted average radius of the particles in each of the five size groups is

$$r_{ij} = \frac{\int_{r_i}^{r_j} r \, dn}{\int_{r_i}^{r_j} dn} \quad (i = 1, \dots, 5)(j = i + 1) \quad (4-36)$$

The "self-preserving" particle size distribution is

$$\frac{dn}{dr} = 0.05 \, \phi r^{-4} . \quad (4-2)$$

Substituting this into Equation (4-36) gives

$$r_{ij} = \frac{\int_{r_i}^{r_j} 0.05\phi r^{-3} dr}{\int_{r_i}^{r_j} 0.05\phi r^{-4} dr} \quad (4-37)$$

$$= \frac{\int_{r_i}^{r_j} r^{-3} dr}{\int_{r_i}^{r_j} r^{-4} dr} \quad (4-38)$$

Integrating between the indicated limits

$$r_{ij} = \frac{-\frac{1}{2}\left(\frac{1}{r_j^2} - \frac{1}{r_i^2}\right)}{-\frac{1}{3}\left(\frac{1}{r_j^3} - \frac{1}{r_i^3}\right)} \quad (4-39)$$

or, since $r_j > r_i$

$$r_{ij} = 1.5 \frac{\left(\frac{1}{r_i^2} - \frac{1}{r_j^2}\right)}{\left(\frac{1}{r_i^3} - \frac{1}{r_j^3}\right)} \quad (4-40)$$

This equation can be rearranged in the following manner:

$$r_{ij} = 1.5 \frac{\left(\frac{r_j^2 - r_i^2}{r_i^2 r_j^2} \right)}{\left(\frac{r_j^3 - r_i^3}{r_i^3 r_j^3} \right)} \quad (4-41)$$

$$= 1.5 \frac{\left(\frac{r_j^2 - r_i^2}{r_j^3 - r_i^3} \right) (r_i r_j)}{1} \quad (4-42)$$

The particle balances on each of the five size groups considered are shown in Figure 4-5. Only one of the five particle balance equations will be used to illustrate how the transfer or agglomeration terms are eliminated. Consider the particle balance equation for particle size group 3, which contains particles with radii ranging from a minimum of r_3 to a maximum of r_4 , with an average radius of r_{34} :

$$\frac{\partial n_{34}}{\partial t} = S_{34} + (A_{-1,3} + A_{-2,3}) - (A_{-3,4} + A_{-3,5}) - \quad (4-43)$$

$$R_{S,34} - P_{P,34}$$

where

n_{34} = the number of particles with an average radius of r_{34} (ranging from r_3 to r_4) present in a unit volume of aerosol suspended in the cask, particles/cm³ aerosol in cask,

S_{34} = the rate at which particles with an average radius of r_{34} are added to the size group upon bursting of the fuel pins (or oxidation of fuel), particles/cm³ aerosol in cask x sec.

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FIGURE 4-5. Particle Balances on Size Groups and Illustration of Particle Flow Between Groups.

$R_{S,34}$ = the rate at which particles with an average radius of r_{34} are removed from the size group by settling, particles/cm³ aerosol in cask x sec.

$R_{P,34}$ = the rate at which particles with an average radius of r_{34} are removed from the size group by plateout, particles/cm³ aerosol in cask x sec.

$A_{-1,3}$ and $A_{-2,3}$ = the rates of formation of particles of average radius r_{34} in size group 3 by agglomeration of smaller particles from size groups 1 and 2, respectively, particles/cm³ aerosol in cask x sec.

$A_{-3,4}$ and $A_{-3,5}$ = the rates at which particles of average radius r_{34} in size group 3 are lost from size group 3 by agglomeration to yield the larger particles of size groups 4 and 5, respectively, particles/cm³ aerosol in cask x sec.

The transfer rates $A_{-1,3}$, $A_{-2,3}$, $A_{-3,4}$, and $A_{-3,5}$ may be eliminated from Equation (4-43) if it is assumed that they are such that the self-preserving particle size distribution is maintained throughout the life of the aerosol. Using this assumption, the particle balance equation reduces to

$$\frac{dn_{34}}{dt} = S_{34} - R_{S,34} - R_{P,34} \quad (4-44)$$

where it is to be noted that the accumulation or storage rate is no longer a partial derivative with respect to time.

Since n_{34} is the number of particles of average radius r_{34} present in a unit volume of aerosol in the cask, then the total particles of this size in the cask would be

$$N_{34} = n_{34} V_{CSK} \quad (4-45)$$

where

V_{CSK} = the total free volume in the cask, cm^3 .

It is assumed that the total volume of the aerosol in the cask is the total free volume in the cask containment.

Substituting the source rate and removal rate terms defined by Equations (4-25), (4-6) and (4-23) into Equation (4-44) gives

$$\frac{dn_{34}}{dt} = n_{S34} \frac{V_N}{V_{CSK}} \delta(t) - \frac{n_{34} V_{f34} A_f}{V_{CSK}} - \frac{D_{P34} A_{SURF} n_{34}}{\delta V_{CSK}}. \quad (4-46)$$

The loss-of-coolant model of the IF-300 consists of numerous nodes or regions connected by admittances that represent the cask as an analogous electrical network (see Figure 3-20). Seven of these nodes represent the spent fuel assemblies. Each of these seven nodes is a potential source of particles. Consequently, Equation (4-46) may be modified as follows:

$$\begin{aligned} \frac{dn_{34}}{dt} = & \sum_{k=1}^7 n_{S,34k} \frac{V_{Nk}}{V_{CSK}} \delta_k(t) - \frac{n_{34} V_{f34} A_f}{V_{CSK}} \\ & - \frac{D_{P34} A_{SURF} n_{34}}{\delta V_{CSK}} \end{aligned} \quad (4-47)$$

where

k = the number of fuel nodes.

The variables n_{34} and $n_{S,34k}$ in this equation represent the number of particles in the size range r_3 to r_4 so, in a spatial sense, they may be considered to be increments. Therefore, an approximate value for these variables may be obtained from the self-preserving particle size distribution

function, which expresses the variation of the number of particles in an aerosol with respect to particle radius

$$\frac{dn}{dr} = 0.05 \phi r^{-4} . \quad (4-2)$$

For the increment of particle size radius beginning with r_3 and ending with r_4 , we can write the approximations:

$$\frac{n_{34}}{(r_4 - r_3)} = 0.05 \phi r_3^{-4} . \quad (4-48)$$

and

$$\frac{n_{S,34k}}{(r_4 - r_3)} = 0.05 \phi_k r_3^{-4} . \quad (4-49)$$

It should be recalled that the subscripts on the variables n_{34} and $n_{S,34k}$ signify that this is the number of particles in the size range r_3 to r_4 , but that a weighted average radius was used for the particles rather than trying to cope with a range of radii [see Equations (4-36) through (4-42)]. A weighted average radius was necessary to calculate the volume of the particles in a size group. This would not have been possible if only the number of particles in a size range were determined, because there would be no way of knowing the actual numbers and sizes of the particles in the size group.

The volume fraction of the disperse phase of the aerosol in the cask is

$$\phi = \frac{V_P}{V_{CSK}} \quad (4-50)$$

where

V_P = the volume of all the particles in all the size groups in the aerosol in the cask, cm^3 of particles in the cask,

V_{CSK} = the free volume inside the cask and also the volume of the aerosol in the cask containing particles in all the size groups, cm^3 of aerosol in the cask.

The volume fraction of the disperse phase of the aerosol contained in the k-th fuel node is:

$$\phi_k = \frac{V_{Pk}}{V_{Nk}} \quad (4-51)$$

[See Section 4.2 Equation (4-95)]

where

V_{Pk} = the volume of all the particles in all the size groups contained in the k-th fuel node, cm^3 of particles in the k-th fuel node,

V_{Nk} = the volume of the aerosol in the k-th fuel node, cm^3 of aerosol in k-th fuel node.

Combining Equation (4-48) and Equation (4-50) and rearranging yields

$$n_{34} = 0.05 \frac{V_P}{V_{CSK}} (r_4 - r_3) r_3^{-4} . \quad (4-52)$$

Similarly, Equations (4-49) and (4-51) may be combined to give

$$n_{S,34k} = 0.05 \frac{V_{Pk}}{V_{Nk}} (r_4 - r_3) r_3^{-4} . \quad (4-53)$$

The total number of particles with an average radius of r_{34} has been expressed as Equation (4-45)

$$N_{34} = n_{34} V_{CSK} . \quad (4-45)$$

Applying the same relationship to the k-th fuel node gives the following equation for the total number of particles of this size in the aerosol released from the k-th fuel node

$$N_{S,34k} = n_{S,34k} V_{Nk} \quad (4-54)$$

Multiplying Equation (4-47) by V_{CSK} and applying (4-45) and (4-54) gives

$$\frac{dN_{34}}{dt} = \sum_{k=1}^7 N_{S,34k} \delta_k(t) - \frac{V_{f34} A_f N_{34}}{V_{CSK}} - \frac{D_{P34} A_{SURF} N_{34}}{\delta V_{CSK}} \quad (4-55)$$

or

$$\frac{dN_{34}}{dt} = \sum_{k=1}^7 N_{S,34k} \delta_k(t) - \left(\frac{V_{f34} A_f}{V_{CSK}} + \frac{D_{P34} A_{SURF}}{\delta V_{CSK}} \right) N_{34} \quad (4-56)$$

Also, applying Equations (4-45) and (4-54) to Equations (4-52) and (4-53), respectively, yields

$$N_{34} = 0.05 V_P (r_4 - r_3) r_3^{-4} \quad (4-57)$$

and

$$N_{S,34k} = 0.05 V_{Pk} (r_4 - r_3) r_3^{-4} \quad (4-58)$$

Setting

$$C_{34} = \frac{V_{f34} A_f}{V_{CSK}}, \quad (4-59)$$

$$D_{34} = \frac{D_{P34} A_{SURF}}{\delta V_{CSK}}, \quad (4-60)$$

and

$$CD_{34} = C_{34} + D_{34}, \quad (4-61)$$

Equation (4-56) can be written as

$$\frac{dN_{34}}{dt} = \sum_{k=1}^7 N_{S,34k} \delta_k(t) - CD_{34} N_{34} . \quad (4-62)$$

Substituting from Equations (4-57) and (4-58) into Equation (4-62) gives:

$$\frac{dN_{34}}{dt} = 0.05 (r_4 - r_3) r_3^{-4} \sum_{k=1}^7 V_{Pk} \delta_k(t) - 0.05 CD_{34} V_P (r_4 - r_3) r_3^{-4} . \quad (4-63)$$

Setting

$$A_{34} = 0.05 CD_{34} (r_4 - r_3) r_3^{-4} , \quad (4-64)$$

and

$$B_{34} = 0.05 (r_4 - r_3) r_3^{-4} , \quad (4-65)$$

Equation (4-63) may be written as

$$\frac{dN_{34}}{dt} = B_{34} \sum_{k=1}^7 V_{Pk} \delta_k(t) - A_{34} V_P . \quad (4-66)$$

The total volume of the particles in the aerosol in the cask is

$$V_P = \frac{4}{3} \pi (r_{12}^3 N_{12} + r_{23}^3 N_{23} + r_{34}^3 N_{34} + r_{45}^3 N_{45} + r_{56}^3 N_{56}) , \quad (4-67)$$

and the total volume of the particles in the aerosol in the k-th fuel node is

$$V_{Pk} = \frac{4}{3} \pi (r_{12}^3 N_{12} + r_{23}^3 N_{23} + r_{34}^3 N_{34} + r_{45}^3 N_{45} + r_{56}^3 N_{56})_k . \quad (4-68)$$

Finally, substituting these particle volumes in Equation (4-66) gives

$$\begin{aligned} \frac{dN_{34}}{dt} = & B_{34} \sum_{k=1}^7 \frac{4}{3} \pi (r_{12}^3 N_{12} + r_{23}^3 N_{23} + r_{34}^3 N_{34} + r_{45}^3 N_{45} + r_{56}^3 N_{56})_k \delta_k(t) \\ & - \frac{4}{3} \pi A_{34} (r_{12}^3 N_{12} + r_{23}^3 N_{23} + r_{34}^3 N_{34} + r_{45}^3 N_{45} + r_{56}^3 N_{56}) . \end{aligned} \quad (4-69)$$

In general, the modified particle balance equation for particles in the size range r_i to r_j may be written as

$$\frac{dN_{ij}}{dt} = B_{ij} \sum_{k=1}^K \left[\sum_{i=1}^{N_{GPS}} \frac{4}{3} \pi (r_{ij}^3 N_{ij}) \right]_k \delta_k(t) - \frac{4}{3} \pi A_{ij} \sum_{i=1}^{N_{GPS}} r_{ij}^3 N_{ij} \quad (4-70)$$

where

$$i = 1, 2, 3, \dots, N_{GPS} ,$$

$$j = i + 1$$

$$k = 1, 2, \dots, K$$

and, in the present study,

$$N_{GPS} = 5$$

and

$$K = 7.$$

The derivation of Equations (4-69) and (4-70) shows that, if it is assumed that (1) the agglomeration terms (terms which represent the rate of

transfer of particles from one size group to another) are such that a self-preserving particle size distribution is maintained throughout the life of the aerosol, and that (2) the same self-preserving particle size distribution holds for any quantities of aerosol which may be added to or removed from the main aerosol, then the agglomeration terms may be removed from the general particle balance of Equation (4-1). The number of particles in any one size group retains its influence on the number of particles present in the other size groups through the particle size distribution function factored into the source and removal terms in the respective particle balance equations.

Integration of Equation (4-69) yields

$$\int_0^{N_{34}} dN_{34} = \int_0^t B_{34} \sum_{k=1}^7 \frac{4}{3} \pi (r_{12}^3 N_{12} + \dots + r_{34}^3 N_{34} + \dots + r_{56}^3 N_{56})_k \delta_k(t) dt$$

$$- \int_0^t \frac{4}{3} \pi A_{34} (r_{12}^3 N_{12} + \dots + r_{34}^3 N_{34} + \dots + r_{56}^3 N_{56}) dt$$

(4-71)

or

$$N_{34} = B_{34} \sum_{k=1}^7 \frac{4}{3} \pi (r_{12}^3 N_{12} + \dots + r_{56}^3 N_{56})_k H_k(t) - \int_0^t (\text{LOSS})_{34} dt.$$

(4-72)

The integration of Equation (4-70) yields

$$N_{ij} = B_{ij} \sum_{k=1}^K \left[\sum_{i=1}^{N_{GPS}} \frac{4}{3} \pi (r_{ij}^3 N_{ij}) \right]_k H_k(t) - \int_0^t (\text{LOSS})_{ij} dt$$

(4-73)

where

$$(\text{LOSS})_{ij} = \frac{4}{3} \pi A_{ij} \sum_{i=1}^{N_{\text{GPS}}} (r_{ij}^3 N_{ij}) \quad (4-74)$$

$$i = 1, 2, 3, \dots, N_{\text{GPS}}$$

$$j = i + 1$$

$$k = 1, 2, \dots, K.$$

Setting

$$NIN_{ij} = B_{ij} \sum_{k=1}^K \left[\sum_{i=1}^{N_{\text{GPS}}} \frac{4}{3} \pi (r_{ij}^3 N_{ij}) \right] H_k(t), \quad (4-75)$$

and

$$NOUT_{ij} = \int_0^t (\text{LOSS})_{ij} dt, \quad (4-76)$$

the integrated particle balance equation becomes

$$N_{ij} = NIN_{ij} - NOUT_{ij}. \quad (4-77)$$

The unit functions $H_k(t)$ are represented in the simulation model by the fuel pin clad burst switches BSW_k and the fuel oxidation switches OSW_k, where k denotes the k -th fuel node (see Figures 4-1 and 4-2).

The total mass of the particles in the aerosol remaining in suspension in the cask is:

$$MASS = \sum_{i=1}^{N_{\text{GPS}}} M_{ij} N_{ij}, \quad (4-78)$$

and the total activity of the particles in suspension is

$$\text{ACTVTY} = \sum_{i=1}^{N_{\text{GPS}}} \text{ACT}_{ij} N_{ij} , \quad (4-79)$$

where

M_{ij} = the mass of an average particle in the size range r_i to r_j , grams/particle

ACT_{ij} = the activity of an average particle in the size range r_i to r_j , curies/particle.

Equations (4-73) through (4-79) are programmed as the transient portion of the simulation model VSØL (see the MIMIC simulation program listing of VSØL in Figure 4-2).

4.1.5 Proposed Modification of the Model to Include Particle Removal by Leakage from the Cask

It was stated earlier that a particle leakage term was not included in the present model but that, since this model was completed, a leakage term has been developed which will be included in the model during the next development phase. The development of this leakage term and the procedure for adding it to the present model are presented in this section.

The key variable in the proposed leakage term is the velocity of the mixture of residual coolant vapor and fission gases flowing from the breach opened in the cask containment at impact. This velocity will be obtained from proposed additions to the Loss-of-Coolant models described in Section 3. The proposed modifications to the Loss-of-Coolant models are presented in Section 3.5.3. The velocity of the gas mixture leaking from the gap is defined by Equation (3-102).

4.1.5.1 Particle Removal by Leakage

The term for particle removal from the aerosol in the cask by leakage is very similar to the term for particle removal by settling. Like the settling term, the leakage term is based on the assumption that the aerosol in the cask is well-stirred, i.e., that the concentration of particles in

each of the size groups considered is the same everywhere in the free volume in the cask. Also, it is assumed that this applies to the gas volume flowing through the breach.

Consider a particle balance on the size group containing particles with an average radius of r_{ij} , with no source of particles and with the only loss of particles due to leakage from the breach.

$$\left[\begin{array}{c} \text{Rate of Change of} \\ \text{Number of Particles} \\ \text{in the Size Group} \end{array} \right] = \left[\text{Input Rate} \right] - \left[\text{Output Rate} \right] \quad (4-80)$$

or

$$\frac{dn_{ij}}{dt} = 0 - R_{Lij} \quad (4-81)$$

where

R_{Lij} = the rate at which particles with an average radius of r_{ij} are removed from the aerosol due to leakage from the breach, particles/cm³ aerosol x sec.

The rate at which the particles pass through the breach and escape from the cask is

$$R_{Lij} = \frac{n_{ij} u A_{GAP}}{V_{CSK}} \quad (4-82)$$

where

u = the velocity of the mixture of fission gases and residual coolant vapor flowing through the breach, cm/sec,

A_{GAP} = the cross-sectional or flow area of the breach, cm^2 .

It is assumed that the particles will be traveling at the same velocity as the gas mixture, i.e., there is no slip or drag.

The particle balance, Equation (4-81), may now be written as

$$\frac{dn_{ij}}{dt} = \frac{n_{ij} u A_{GAP}}{V_{CSK}} \quad (4-83)$$

The velocity u is defined by Equation (3-102) of Section 3.5.3

$$u = \frac{D_{GAP}^2 g_c \left(\frac{mRT_{CSK}}{V_{CSK} f_m} - P_{ATM} \right)}{32 \mu L_{GAP}} \quad (3-102)$$

4.1.5.2 Modification of the Particle Balance Equations and the Model to Include the Leakage Term

There are five particle balance equations in the model, one for each of five particle size groups considered. In Section 4.1.4, only one of these was used to illustrate how the transfer or agglomeration terms are eliminated. The same approach will be used here to show how the particle balance equations will be modified to include the leakage term of Equation (4-83).

Consider the reduced particle balance equation for particle size group 3, which contains particles with radii ranging from a minimum of r_3 to a maximum of r_4 , with an average radius of r_{34} :

$$\frac{dn_{34}}{dt} = S_{34} - R_{S,34} - R_{P,34} \quad (4-44)$$

This equation is a reduced form of Equation (4-43), which includes agglomeration terms. It was assumed that the agglomeration terms could be eliminated if they were such that the self-preserving particle size distribution [see Equation (4-2)] is maintained throughout the life of the aerosol.

Including the loss rate due to leakage, Equation (4-44) is changed to:

$$\frac{dn_{34}}{dt} = S_{34} - R_{S,34} - R_{P,34} - R_{L,34} \quad (4-84)$$

Substituting the source rate term defined by Equation (4-25), and the settling, plateout and leakage removal rate terms defined by Equations (4-6), (4-23), and (4-83), respectively, into Equation (4-84) gives

$$\frac{dn_{34}}{dt} = n_{S,34} \frac{V_N}{V_{CSK}} \delta(t) - \frac{n_{34} V_{f34} A_f}{V_{CSK}} - \frac{D_{P34} A_{SURF} n_{34}}{V_{CSK}} - \frac{n_{34} u A_{GAP}}{V_{CSK}} \quad (4-85)$$

Since each of the seven fuel nodes in the loss-of-coolant model of the IF-300 is a potential source of particles, the source term is written in a form to include all the fuel nodes, and Equation (4-85) becomes

$$\frac{dn_{34}}{dt} = \sum_{k=1}^7 n_{S,34k} \frac{V_{Nk}}{V_{CSK}} \delta_k(t) - \frac{n_{34} V_{f34} A_f}{V_{CSK}} - \frac{D_{P34} A_{SURF} n_{34}}{V_{CSK}} - \frac{n_{34} u A_{GAP}}{V_{CSK}} \quad (4-86)$$

The total number of particles in the aerosol in the cask, with an average radius r_{34} , has been defined by Equation (4-45) in Section 4.1.4 as

$$N_{34} = n_{34} V_{CSK} \quad (4-45)$$

Similarly, the total number of particles of this size in the aerosol released from the k-th fuel node has been defined as

$$N_{S,34k} = n_{S,34k} V_{Nk} . \quad (4-54)$$

Multiplying Equation (4-86) by V_{CSK} , applying (4-45) and (4-54), and rearranging, gives

$$\frac{dN_{34}}{dt} = \sum_{k=1}^7 N_{S,34k} \delta_k(t) - \left(\frac{V_{f34} A_f}{V_{CSK}} + \frac{D_{P34} A_{SURF}}{\delta V_{CSK}} + \frac{u A_{GAP}}{V_{CSK}} \right) N_{34} . \quad (4-87)$$

From Section 4.1.4,

$$C_{34} = \frac{V_{f34} A_f}{V_{CSK}} \quad (4-59)$$

and

$$D_{34} = \frac{D_{P34} A_{SURF}}{\delta V_{CSK}} . \quad (4-60)$$

Setting

$$L_{34} = \frac{u A_{GAP}}{V_{CSK}} \quad (4-88)$$

and

$$CD_{34} = C_{34} + D_{34} + L_{34} , \quad (4-89)$$

Equation (4-87) may be written as

$$\frac{dN_{34}}{dt} = \sum_{k=1}^7 N_{S,34k} \delta_k(t) - CD_{34} N_{34} , \quad (4-90)$$

which is the same as Equation (4-62) in Section 4.1.4. The development of this equation to the final form used [Equation (4-69)], and to the general equation for all size groups [Equation (4-70)], is carried out as outlined earlier in the remainder of Section 4.1.4.

The modification of the general particle balance equation, and of the model, to include a term for particle removal by leakage turns out to be quite simple. The leakage term only changes the equation for CD_{ij} . An additional slight change would have to be made to the model to input the velocity u as a function of time, as obtained from the loss-of-coolant model.

4.2 Supplementary Equations and Procedures

4.2.1 The Volume Fraction of the Disperse Phase of the Aerosol Contained in the k-th Fuel Node

The number of fuel pins in the k-th fuel node (in this case, representing seven fuel assemblies) is

$$P_k = N_{PINS} S_k \quad (4-91)$$

where

- P_k = the number of fuel pins in node k, pins/node,
- N_{PINS} = the number of pins in a unit area of fuel assembly,
pins/cm²,
- S_k = the cross-sectional area of fuel assembly in fuel
node k, cm² assembly/node.

The volume of volatile solids or solid fission products in the k-th fuel node is

$$V_{Pk} = V_{PIN} P_k \quad (4-92)$$

where

- V_{Pk} = the volume of volatile solids in the k-th fuel node,
cm³ particles/node,
- V_{PIN} = the volume of volatile solids in a pin, cm³-particles/
pin.

The volume of void space in the fuel pins in the k-th node is

$$V_{Gk} = P_k \text{VOID} \quad (4-93)$$

where

V_{Gk} = the volume of void space in the pins in the k-th node, cm^3 of void space/node,

VOID = the volume of void space in a fuel pin, cm^3 of void space/pin.

The total volume of aerosol in all the fuel pins in the k-th node is

$$V_{Nk} = V_{Gk} + V_{Pk} \quad (4-94)$$

where

V_{Nk} = the total volume of aerosol in the k-th fuel node, cm^3 aerosol in the k-th node.

Finally, the volume fraction of the disperse phase of the aerosol contained in the k-th fuel node is

$$\phi_k = \frac{V_{Pk}}{V_{Nk}}. \quad (4-95)$$

4.2.2 Calculation of the Volume, Mass and Activity of Average Particles in the Size Range r_i to r_j

4.2.2.1 The Weighted Average Volume

The determination of the mass and activity of a particle in the size range r_i to r_j was based on a weighted average volume, since this produced slightly higher values than those obtained using the weighted average radius of Equation (4-42). The weighted average volumes determined by the method in this section were about 22 percent higher in the size group containing the smallest particles and about 0.3 percent higher in the size group containing the largest particles.

The weighted average volume, using the weighted average radius of Equation (4-42), was determined from Equation (4-96),

$$V_{ij} = \frac{4}{3} \pi r_{ij}^3 . \quad (4-96)$$

The weighted average volume used in the model was based on the assumption that the volume could be weighted according to the number of particles of each size present in the range considered, as shown in Equation (4-97),

$$V_{ij} = \frac{\int_{r_i}^{r_j} V dn}{\int_{r_i}^{r_j} dn} \quad (4-97)$$

where

V_{ij} = the average volume of the particles in the size range r_i to r_j , weighted according to the number of particles of each size present in the range, $\text{cm}^3/\text{particle}$,

V = the volume of a particle, $\text{cm}^3/\text{particle}$,

n = the number of particles of volume V , particles.

The volume V of a particle, assumed to be spherical, is

$$V = \frac{4}{3} \pi r^3 . \quad (4-98)$$

Using the self-preserving particle size distribution function, Equation (4-2), and Equation (4-98), Equation (4-97) may be rewritten as

$$V_{ij} = \frac{\int_{r_i}^{r_j} \left(\frac{4}{3} \pi r^3\right) (0.05 \phi r^{-4} dr)}{\int_{r_i}^{r_j} (0.05 \phi r^{-4} dr)} \quad (4-99)$$

or

$$V_{ij} = \frac{\frac{4}{3} \pi \int_{r_i}^{r_j} \frac{dr}{r}}{\int_{r_i}^{r_j} r^{-4} dr} \quad (4-100)$$

Finally, carrying out the integrations in Equation (4-100), the weighted average volume becomes

$$V_{ij} = \frac{4 \pi \ln \frac{r_j}{r_i}}{\left(\frac{1}{r_i^3} - \frac{1}{r_j^3}\right)} \quad (4-101)$$

4.2.2.2 Calculation of the Mass and Activity of an Average Particle

Of all the potentially volatile solids in PWR fuel, there is more cesium present than all the others combined. This cesium is not present as the metal, but probably exists as various chemical compounds, including several oxides, the molybdenite, the iodide, the uranate and diuranate, and the zirconate. The temperature at which the pins burst, following loss of primary coolant from the IF-300, is about 921°F and the pressure is about 1896 psia. It was assumed that, when the pins burst, particles

of these compounds would be released with the fission gases. Since the relative amounts of the compounds present were unknown, it was convenient to assume that they could be considered to be the oxide, Cs_2O .

Experimental data show that it is unlikely that more than one percent of the total cesium in all of the fuel pins will migrate to the pin void space during reactor operation and that, of this amount, less than one percent would be released under conditions postulated to occur in a severe transportation accident.

General Electric's analysis of the release of fission products from the spent fuel in the IF-300⁽¹⁾ was limited to the release of the fission gases I, Kr, and Xe; consequently, the fission product inventories presented in Reference (1) did not include cesium. An estimate of the amount of cesium present in the PWR spent fuel was derived from fission product inventories for spent Diablo Canyon reference fuel that had been cooled 90 days.⁽¹⁴⁾ A small correction factor was applied to these data to account for differences in exposure. The fission product inventories for the Design Basis PWR 1 spent fuel of Reference (1), and the spent Diablo Canyon reference fuel of Reference (14) are compared in Table 3-1.

The mass and activity of the cesium are calculated as follows. From Table 3-1, the mass of the cesium in the Design Basis PWR 1 spent fuel is about $2910 \frac{\text{grams}}{\text{MTU}}$, the mass of uranium in a fuel assembly is 457 kgU, and the number of PWR fuel assemblies carried by the IF-300 is 7. Therefore, the mass of the cesium in the cask is

$$\begin{aligned} M(\text{Cs}) &= \left(2910 \frac{\text{grams}}{\text{MTU}} \right) \left(\frac{\text{MTU}}{10^3 \text{ kgU}} \right) \left(457 \frac{\text{kgU}}{\text{Assembly}} \right) (7 \text{ assemblies}) \\ &= 9310 \text{ grams.} \end{aligned}$$

Also, from Table 3-1, the activity of the cesium in the Design Basis fuel is about $353,000 \frac{\text{Ci}}{\text{MTU}}$. Therefore, the activity of the cesium in the cask is

$$\begin{aligned} A(\text{Cs}) &= \left(353,000 \frac{\text{Ci}}{\text{MTU}} \right) \left(\frac{\text{MTU}}{10^3 \text{ kgU}} \right) \left(457 \frac{\text{kgU}}{\text{Assembly}} \right) (7 \text{ assemblies}) \\ &= 1.13 \times 10^6 \text{ Ci.} \end{aligned}$$

It was assumed that the cesium is released from the fuel pins as the oxide Cs_2O . The atomic weight of Cs is $133 \frac{\text{grams}}{\text{gram-atom}}$, and the molecular weight of Cs_2O is $282 \frac{\text{grams}}{\text{gram-mole}}$. Therefore, if all the cesium in the fuel in the cask is assumed to be in the form of Cs_2O , the mass of the oxide in the cask would be

$$M(\text{Cs}_2\text{O}) = \frac{(9310 \text{ grams})(282)}{(2)(133)} = 9870 \text{ grams} .$$

The number of curies in a gram of Cs_2O is

$$C_{\text{PM}} = \frac{1.13 \times 10^6 \text{ Ci}}{9870 \text{ grams } \text{Cs}_2\text{O}} = 114.6 \frac{\text{curies}}{\text{gram}} .$$

Less than one percent of the total cesium in the fuel will migrate to the pin voids during reactor operation, and only one percent of this amount will be released when the fuel pins burst. Therefore, the maximum amount of Cs_2O that might be released from the spent fuel would be

$$M_{\text{TOTIN}} = (0.0001)M(\text{Cs}_2\text{O}) = 0.987 \text{ grams}$$

with a total activity of

$$A_{\text{TOTIN}} = (0.0001)A(\text{Cs}) = 113 \text{ curies} .$$

The mass of an average particle of Cs_2O in the size range r_i to r_j would be

$$M_{ij} = \rho V_{ij} \quad (4-102)$$

where

$$M_{ij} = \text{the mass of the average particle, } \frac{\text{grams}}{\text{particle}} ,$$

V_{ij} = the weighted average volume of the average particle as defined by Equation (4-101), $\text{cm}^3/\text{particle}$,
 ρ = the density of Cs_2O , grams/cm^3 .

The activity of an average particle in the size range r_i to r_j would be

$$\text{ACT}_{ij} = C_{PM} M_{ij} . \quad (4-103)$$

4.2.2.3 Correction Factor Required for the Calculation of the Mass and Activity of an Average Particle

The number of particles in the size range r_i to r_j present as an aerosol in the k -th fuel node is obtained from the following form of the self-preserving particle size distribution function

$$N_{ijk} = 0.05 \phi_k V_{Nk} N_{ASSY} r_i^{-4} (r_j - r_i) , \quad (4-104)$$

$$(i = 1, \dots, 5)(j = i + 1)(k = 1, \dots, K)$$

where

N_{ijk} = the number of particles in the size range r_i to r_j present in the k -th fuel node, particles, $= n_{ijk} V_{Nk}$,

ϕ_k = the volume fraction of the disperse phase of the aerosol in the k -th fuel node [See Equation (4-95)],
 $\frac{\text{cm}^3 \text{ of particles in } k\text{-th fuel node}}{\text{cm}^3 \text{ of aerosol in } k\text{-th fuel node}}$,

V_{Nk} = the volume of the aerosol in the k -th fuel node,
 cm^3 aerosol in the k -th fuel node,

N_{ASSY} = the number of fuel assemblies in the cask.

The total mass of the particles available in all the size groups and fuel nodes would be

$$M_{TOT} = \sum_{i=1}^{N_{GPS}} \sum_{k=1}^K N_{ijk} M_{ij} , \quad (4-105)$$

$$(i = 1, \dots, N_{GPS})(j = i + 1)(k = 1, \dots, K) .$$

When the total mass of the Cs_2O calculated from Equation (4-105) was compared with the known mass, M_{TOTIN} , they were not the same. After a study of all the factors involved, it was concluded that the difference was somehow due to the discretization or lumping of the particles into size increments and representing them by a weighted average radius and volume. It was decided that the simplest way to correct the discrepancy would be to apply a correction factor based on the difference between M_{TOTIN} and M_{TOT} .

The correction factor, FACT, was defined as shown in Equation (4-106):

$$FACT = 1 + \frac{M_{TOTIN} - M_{TOT}}{M_{TOTIN}} . \quad (4-106)$$

M_{TOT} is repeatedly calculated at time zero, using Equations (4-101), (4-102), (4-104) and (4-105), and compared to M_{TOTIN} . As long as

$$|M_{TOTIN} - M_{TOT}| < 1 , \quad (4-107)$$

the simulation time is held at zero and the correction factor of Equation (4-106) is applied. As soon as

$$|M_{TOTIN} - M_{TOT}| \geq 1 , \quad (4-108)$$

the iteration is stopped, the last value of M_{TOT} accepted, and the simulation time advanced.

Unfortunately, the correction factor FACT was applied to Equation (4-104), which alters the number of particles injected into the aerosol from

the fuel regions. This implies that the self-preserving particle size distribution function somehow is in error. This is unfortunate since this distribution function is believed to be a valid representation of the particle size distribution in the aerosol produced. The correction factor should have been applied to the weighted average volume defined by Equation (4-101). The weighted average volume of particles in the size range r_i to r_j is based on the discretization or lumping of the particles into several size groups. This lumping of particles into size groups, where the particles are assigned an average radius and volume, is believed to be the source of the difference between the calculated and known total mass of the cesium. A simple readjustment will be made later in the simulation model to apply the correction factor to the weighted average volume rather than to the number of particles in a size group.

The total activity of the particles available in all the size groups and fuel nodes would be

$$A_{TOT} = \sum_{i=1}^{N_{GPS}} \sum_{k=1}^K N_{ijk} ACT_{ij} \quad (4-109)$$

$$(i = 1, \dots, N_{GPS})(j = i + 1)(k = 1, \dots, K)$$

or

$$A_{TOT} = C_{PM} M_{TOT} \quad (4-110)$$

4.2.2.4 Calculation of the Number of Average Particles Available: Total, Free and Bound up

The total number of particles in the size range r_i to r_j available as an aerosol in the k -th fuel node is obtained from Equation (4-104) (see Section 4.2.2.3)

$$N_{ijk} = 0.05 \phi_k V_{N_k} N_{ASSY} r_i^{-4} (r_j - r_i) . \quad (4-104)$$

The total number of free particles, in the size range r_i to r_j in the void spaces of the fuel pins in the k-th node, released when the pin clads burst is

$$N_{Bijk} = F_R F_{SOL} N_{ijk} \quad (4-111)$$

where

F_{SOL} = the fraction of the inventory of the total cesium in the fuel that migrates to the pin voids during reactor operation,

F_R = the fraction of the cesium migrated to the pin voids that is released with the fission gases when the pin clads burst.

The total number of particles in the size range r_i to r_j in the k-th fuel node, bound up in the fuel and released only after the fuel is oxidized to the granular U_3O_8 , is

$$N_{OXijk} = F_R (1 - F_{SOL}) N_{ijk} \quad (4-112)$$

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