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A SCOPING STUDY OF FISSION PRODUCT
TRANSPORT FROM FAILED FUEL DURING
N REACTOR POSTULATED ACCIDENTS

D. L. Hagrman

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FROM FAILED FUEL DURING N REACTOR POSTULATED ACCIDENTS

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ABSTRACT

This report presents a scoping study of cesium, iodine, and tellurium behavior during a cold leg manifold break in the N Reactor. More detail about fission product behavior than has previously been available is provided and key parameters that control this behavior are identified. The LACE LAI test and evidence from the Power Burst Facility Severe Fuel Damage tests are used to test the key model applied to determine aerosol behavior. Recommendations for future analysis are also provided. The primary result is that most of the cesium, iodine, and tellurium remains in the molten uranium fuel. Only 0.0035 of the total inventory is calculated to be released. Condensation of most of the species of cesium and iodine that are released is calculated, with 0.998 of the released cesium and iodine condensing in the spacers and upstream end of the connector tubes. Most of the tellurium that is released condenses but the chemical reaction of tellurium vapor with surfaces is also a major factor in the behavior of this element.

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EXECUTIVE SUMMARY

In response to questions about fission product behavior in the N Reactor, studies with detailed nuclear fuel behavior codes have been initiated. This report presents a parallel scoping study designed to direct the studies with detailed codes to key areas and to provide early results for one of the scenarios under investigation, the cold leg manifold break.

Results from a companion RELAP5 study and other sources were employed as thermal-hydraulic boundary conditions but no model for fuel behavior was available so some model development was necessary. A model for the release of fission products under isothermal conditions was modified so that it could be applied. The release model is based on fuel oxidation and employs parabolic kinetics (oxidation rate proportional to the inverse of the amount of prior oxidation). Release is therefore concentrated near the time the fuel cladding first ruptures and exposes the metal fuel to steam. It was calculated that only 0.033 of the hot node, hot annular ring inventory is released. This is only 0.0035 of the total inventory.

Concentrations are so low that condensation of the cesium and iodine species, cesium iodine and cesium hydroxide, does not begin until wall temperatures in the 700 to 800 K range are encountered. The corresponding temperatures for tellurium are 550 to 600 K but elemental tellurium reacts chemically in addition to condensing so very little tellurium leaves the volumes considered for any of the temperatures studied in the analysis. No reason for expecting temperatures as high as 700 to 800 K in the connectors has been identified.

In the best estimate case, 0.998 of the released cesium iodide and the released cesium hydroxide is condensed. A total of 0.995 of the released tellurium is removed from the effluent, 0.902 of it by condensation and 0.093 of it by reaction with the walls before it can condense. The mass released from the uranium fuel divided by the mass that leaves the riser is 500, 500, and 1000 for cesium iodide, cesium hydroxide, and tellurium, respectively. If the release fractions are converted to absolute mass by multiplying by the process tube inventory and the number of process tubes, one finds that the calculated releases past the risers are $9 \text{ E-}05 \text{ kg}$ of cesium iodide, $4 \text{ E-}04 \text{ kg}$ of cesium hydroxide, and $8 \text{ E-}06 \text{ kg}$ of tellurium. The results depend on wall temperatures in the process tubes and the connector tubes that lead to the risers. The vapor concentration that is allowed to leave the risers increases about an order of magnitude for every 100 K increase in the wall temperature of the connector tubes. The best estimate temperatures of the spacers and connector tubes are on the order of 500 K so condensation plays a major role at the best estimate temperatures and for assumed wall temperatures up to 200 K higher. Other key parameters are the coolant flow rate and the initial aerosol size. A reduction of the best estimate coolant flow rate by a factor of 0.1 increases fission product concentrations to the point that significant condensation onto pre-existing aerosol seeds can occur. This, in turn, would allow transport of as much as half of some species of released fission products on the smaller aerosols that escape to the risers. Reduction of the estimated radius of the aerosol that is assumed to be present in the process tube by an order of magnitude allows

as much as 0.3 of the released cesium iodide and cesium hydroxide to be transported past the risers as an aerosol.

Less volatile species are not considered explicitly, but their behavior can be inferred from the aerosol behavior calculations because their vapor pressure is too low for significant transport as a vapor. Decontamination factors of approximately 70 are calculated for the best estimate aerosol behavior. When this factor is coupled with release fractions from the fuel of 0.0035, one finds very little release of low volatile fission products.

With the exceptions noted in the preceding paragraphs, aerosol behavior is not found to be very important in the analysis of the cold leg manifold break scenario for the N Reactor. In the best estimate analysis, the cooling is by heat transfer to a relatively large surface area so that condensation onto the limited aerosol that remains when saturation is exceeded must compete with significant vapor transport to walls that are always a little colder than the aerosol.

Because of the sensitivity of the results to wall temperatures in the spacer regions and connector tubes, it is recommended that future analysis concentrate on obtaining accurate wall temperatures in these regions and on obtaining uncertainty estimates for these temperatures. Another area for additional development is the model for release of fission products from the metal fuel. The model would be more defensible if its uranium oxidation correlation were cast in terms of the surface area exposed to steam. However, this model improvement will only be useful if it can be used with an accurate description of the surface area when the uranium fuel is first exposed to steam. An accurate release model is important because the release rate affects the concentrations and thus the condensation of the fission products. Coolant flow is also an important parameter because it affects the concentrations of the fission products, but the calculations are sensitive to this parameter only if flow is reduced enough (by a factor of ≈ 0.1 times best estimate) to cause condensation onto pre-existing aerosols. Finally, it is recommended that the analysis be repeated with models that calculate the distribution of elements among the possible chemical species as soon as these models are available. It is expected that these models will eliminate the current speculation about the possible effect of a hydrogen environment on the chemical species present.

This report has received independent technical review by M. Epstein of Fauske & Associates, Inc., and the reviewer's comments are attached as Appendix C. The author's response to and resolution of these comments is also attached as Appendix D. Principally, the reviewer suggested the possibility of additional aerosol transport by homogeneously nucleated aerosols formed in the pipe wall boundary layer. The author takes issue in that this extra mode of transport is not patently important, but could be examined in future work for a possible need to include it.

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1. INTRODUCTION

One result of the accident at Chernobyl was a series of questions about fission product behavior in the N Reactor. This report is a first response to those questions and represents a scoping study that can serve to guide more detailed work. It provides more detailed information about the fission product species present and their behavior than has previously been available and it identifies key parameters that control this behavior. Preliminary implications for the N Reactor are reported along with recommendations for any future analysis.

The basis of this study is the cold leg manifold break accident. The pressure tubes, connector piping and riser sections of the reactor were modeled and estimates of the fission product inventory, fission product release rates, aerosol sources, fluid temperatures, coolant flow rates, and wall temperatures were obtained as discussed in Section 2. Many of these data came from a companion study with the RELAP5 computer code¹. Variations in wall temperatures, coolant flow rate, the source rates of aerosols and species vapors, aerosol settling rates, gas composition and the initial aerosol size were considered to help identify important uncertainties.

The analysis was carried out with an analysis tool developed from models in the TRAP-MELT2.0 computer code² to analyze fission product behavior in the Power Burst Facility at the Idaho National Engineering Laboratory during Severe Fuel Damage Tests. The tool calculates fission product behavior in a slug of gas being carried down a long, thin pipe where the more usual assumption of a series of well-mixed volumes connected by junctions is unnecessarily difficult to apply. As in TRAP-MELT2.0, different states of the species are considered. They are aerosol, vapor, aerosol that has been deposited on a surface, condensed on a surface, and chemisorbed on a surface. The aerosol state is partitioned into nineteen size ranges plus an overflow bin for larger sizes. Mass transport between the five states and within the aerosol sub-states due to the coupling mechanisms listed in Table 1.1 are modeled.

Several changes and additions beyond the two coupling mechanisms marked with an asterisk in Table 1.1 were made to the TRAP-MELT2.0 models. Table 1.2 is a summary of these. Table 1.3 is a list of models which are not included. With the exception of a model for turbulent resuspension of deposited aerosols, the models not included are probably not important to this analysis. The likely effect of not modeling resuspension is discussed in Section 3 and tested in Section 6. The analysis tool is designed to employ measurements and thermal-hydraulic calculation results. Table 1.4 is a list of these data and the other input information required to do the analysis.

The next section describes the data and preliminary calculations performed to provide the input data listed in Table 1.4. It is followed by a comparison to some of the LACE LA1 experimental data⁴ to test the aerosol behavior models and their formulation in the analysis tool. Section 4 is a discussion of the modifications required to the analysis tool to treat the N Reactor core. In Section 5, the base case results are discussed. Changes to the base case and their results are presented in

TABLE 1.1 COUPLING MECHANISMS CONSIDERED

Aerosol-to-Deposited Aerosol

- Gravitational Settling
- Thermophoresis
- Diffusion from Turbulent Flow
- Inertial Deposition from Turbulent Flow
- Diffusion from Laminar Flow
- Pipe Bend Deposition*

Aerosol-to-Vapor

- Evaporation/Condensation

Aerosol-to-Aerosol

- Agglomeration due to Brownian Motion
- Agglomeration due to Differential Gravitational Settling
- Agglomeration due to Turbulence
- Evaporation/Condensation

Vapor-to-Condensed

- Evaporation/condensation

Vapor-to-Chemisorbed

- Chemisorbtion (only from vapor to surface. No reverse reactions)

Vapor-to-Deposited Aerosol

- Evaporation*

* These models were not available in TRAP-MELT2.0. They have been added because it was thought they were likely to be important to the test analysis for which the analysis tool was designed

TABLE 1.2. CHANGES AND ADDITIONS TO TRAP-MELT2 MODELS

Generalized Coolant Composition to allow
He, Ar, Kr, Xe, H₂, N₂, O₂, CO, CO₂, and H₂O

Surface Chemisorption on Zircaloy added

Fission Product Heating of Fluid Modeled

Species Extended to Include
H₂Te, HI, Cd, Ag, Sn, SnTe, Condensable H₂O, UO₂ ZrO₂

Simultaneous Solution of Rate Equations

Equilibrium Distribution of Condensate not Assumed for Aerosol Sizes

Time Constants Calculated

Chemisorbtion and Evaporation/Condensation Mass Transport to Surface
Coupled*

CsOH/CsI Surface Interaction Effects on Equilibrium Vapor Pressure
Modeled*

Condensable H₂O Species Considered in Calculating Bulk Coolant
Properties

* These models were provided by personal communication from D. A. Powers of SANDIA National Laboratories, June 5, 1986.³

TABLE 1.3. MODELS NOT INCLUDED

Most Chemical Reactions in the Vapor Phase

(A crude model for $\text{CsOH} + \text{HI} \rightarrow \text{CsI} + \text{H}_2\text{O}$ on cooling is present. No other reactions are considered)

Most Surface State Mixing Effects

(Only CsI/CsOH surface mixing is modeled)

Reversal of Chemisorbtion at Wall Surfaces

Mechanistic CsOH Chemisorbtion by Stainless Steel

(The current model is a constant vapor deposition velocity)

Aerosol/Vapor Chemical Reactions

Turbulent Resuspension of Deposited Aerosols

Aerosol Nucleation from a Vapor

Dissolution of Fission Product Species by Liquid Water

Transport of Condensed Liquids

TABLE 1.4. INFORMATION REQUIRED FOR FISSION PRODUCT BEHAVIOR ANALYSIS

1. Number of major (boundary condition specified) control volumes
2. Number of sub-volumes in each major volume
3. Volume geometry: Length, flow channel cross-sectional area, wall surface area, component of wall surface normal to acceleration of gravity, wall composition (Zircaloy or stainless steel)
4. Angle through which the pipe bends in each subvolume
5. Times at start and end of problem
6. Switch indicating species to be considered
7. Fractional tolerance allowed on states with enough mass to be considered and minimum state mass to be considered in solving differential equations.
8. Print-out frequency and amount selection
9. Mass fractions of key isotopes of chemical species in inventory
10. a) Vapor source rates in first volume for species considered
b) Aerosol Source rate and size distribution in first volume for species considered
11. Tables of noncondensable gas source rates versus time in first volume
12. Table of initial gas temperature versus time in first volume
13. Tables of wall temperatures versus time in all volumes
14. Table of pressure versus time in the first volume
15. Table of shortest boundary conditions change time constant versus time
16. An off-on flag indicating whether debug print-out is desired

Section 6. The final section provides conclusions from this scoping study. These conclusions include both preliminary implications for the N Reactor and recommendations for future analysis.

2. DATA AND PRELIMINARY CALCULATIONS

This section is a description of the derivation of the input data required to carry out the analysis of fission product behavior. Most of the data are provided by the companion study with the RELAP5 computer code¹. However, some data unique to fission product behavior were also required and some of the parameters calculated in the RELAP5 study were modified to be consistent with subsequent results⁵. Since they are not discussed elsewhere, the data not obtained from the RELAP5 study will be discussed in somewhat more detail than the RELAP5 data.

2.1. System Geometry

Table 2.1 is a summary of the dimensions and wall materials of the five major volumes employed to analyze fission product behavior in the N Reactor. The longer volumes were divided into a sufficient number of sub-volumes to allow reasonable modeling of the condensation profile. Figure 2.1 is a scale drawing of the volumes with the lateral dimension scaled one hundred times larger than the dimension along the flow velocity.

Dimensions of the process tubes, connector tubes and risers were taken from the Safety Analysis Report for the N Reactor⁶. The fueled length of the process tubes was represented as three equal lengths, each 3.54 meters. The center and downstream sections of the process tubes were included in the model as volumes 1 and 2. Since the N Reactor fuel has two annular fuel elements and three coolant channels, some modification of the analysis tool or a scaling procedure was required because the analysis tool modeled only a single pipe. The modification option was selected because it is not possible to scale rigorously for both aerosol behavior in the core and condensation behavior downstream. With the modification, the middle flow channel of the three concentric coolant channels (where most of the fission product release occurs) is modeled and the other two parallel channels (the inner circular cross-section and the outer annulus) are treated as a by-pass whose coolant flow is re-introduced in the volume that represents the process tube plenum. The diameters of the circular flow channel boundaries¹ lead to cross-sectional areas of $6.836 \text{ E-}04 \text{ m}^2$ for the channel modeled and $9.335\text{E-}04 \text{ m}^2$ for the bypass channel. (The ratio of these cross-sections is presumed to dictate the partitioning of coolant flow between the bypass and the modeled channel.) The wall surface area and component of wall surface normal to the acceleration of gravity were also calculated from the diameters of the process tube flow channels. The tubes were assumed to be horizontal for the latter calculations so that the net horizontal settling area is the sum of the outside diameter times the length (for the outer wall) plus the inside diameter times the length (for the inside cylinder's surface).

The dimensions of volume 3, the spacer region of the process tube, and volume 4, the connector tube, correspond to the dimensions used in the RELAP5 analysis. The length of volume 3 is equal to the volume/area length of volume 207 (the spacer volume) of the RELAP5 analysis while the

TABLE 2.1. SYSTEM DIMENSIONS AND WALL MATERIALS USED IN THE ANALYSIS

Volume Number	Description	Length <u>(m)</u>	Cross Section <u>(m²)</u>	Wall Surface <u>(m²)</u>	Horizontal Surface <u>(m²)</u>	Wall Type <u> </u>	Pipe Bend <u>(radians)</u>	Number of Subvolumes <u> </u>
1	center 1/3 process tube	3.539	6.836E-04	0.8415	0.2679	Zircaloy	0	2
2	end 1/3 process tube	3.539	6.836E-04	0.8415	0.2679	Zircaloy	0	2
3	spacers	3.797	3.214E-03	0.8105	0.2580	Zircaloy	$\pi/2$	2
4	connector tube	16.80	2.113E-03	2.822	0.8982	Steel	π^1	8
5	riser	7.147	2.005E-03	0.1085	0.2005	Steel	0	4

1. $\pi/2$ radians in the first and last subvolumes

Figure 2.1. Scale drawing of the five main volumes with subvolumes indicated by dashed lines (width scale 100 times length scale).

cross section is the net cross section of the RELAP5 analysis divided by 1003, the number of process tubes.

Surface areas and the horizontal component of surface area were calculated with the assumption that the spacer region of the process tube is a right circular cylinder. A pipe bend of $\Pi/2$ radians in the subvolume at the end of the spacer represents the connection between the spacer region and the connector tube. The length of volume 4 is equal to the volume/area length of volume 208 of the RELAP5 analysis, the connector tube. The cross-sectional area and surface areas were calculated with the same assumptions used for volume 3. Based on drawings from Reference 4, two $\Pi/2$ pipe bends were assumed.

Some scaling assumptions were required for the riser, volume 5, because the coolant from 1003 process tubes is carried to 16 risers. One must use dimensions appropriate to describe one process tube's part of the behavior of a riser. The scaling is designed to be nearly accurate for evaporation and condensation as follows. The total cross section is

$$\text{Total Cross-section} = 16 \Pi r^2 \quad (2.1)$$

where r = the radius of one riser (m). The total surface area is

$$\text{Total Surface} = 16 \ 2\Pi r L \quad (2.2)$$

where L = the length of a riser (m). The cross-section per process tube is

$$\text{Cross-section per process tube} = \frac{16}{1003} \Pi r^2 \quad (2.3)$$

and the surface area per process tube is

$$\frac{16}{1003} \ 2 \Pi r L = \frac{\sqrt{16}}{1003} \ 2L \sqrt{\Pi 16 \Pi r^2} \quad (2.4)$$

that is, the surface area per process tube is

$$\frac{\sqrt{16}}{1003} \ 2L \sqrt{\Pi \text{ Total cross-section}} \quad (2.5)$$

The scaled cross-section of Equation (2.3) and the scaled surface are of Equation (2.5) are used to describe one process tube's part of the behavior in a riser.

The expression used to calculate evaporation or condensation is approximately the TRAP-MELT 2.0 expression,

$$\frac{dC}{dt} = - \frac{A \ 0.023 \ Re^{0.8} \ Sc^{0.33} \ Dv \ (C-C_{eq})}{V \ Dia} \quad (2.6)$$

where

C = species concentration (kg/m^3)
 C_{eq} = equilibrium species concentration over a surface at the given surface temperature (kg/m^3)
 t = time(s)
 A_w = surface area (m^2)
 V = volume of the volume (m^3)
 Re = Reynold's number, density speed Dia / viscosity, (unitless)
 Sc = Schmidt number, viscosity / (density D_v), (unitless)
 D_v = Diffusivity of species vapor in bulk gas (m^2/s)
 Dia = diameter of the pipe (m)

The scaling of Equation (2.3) which is proportional to the cross-section and at constant length causes the scaling to be proportional to the volume-share supplied by each process tube so the correct concentration, C , is employed. The linear scaling of the surface area represented in Equations (2.3) and (2.4) causes the ratio A/V of Equation (2.6) used for each process tube to be the same as the actual A/V ratio in the riser. Thus the only error introduced into Equation (2.6) by using dimensions scaled for individual process tubes is associated with the diameter. Since this factor appears in both the Reynold's number and in the denominator, the ratio of the rate of change of concentration calculated with Equation (2.6) and scaled quantities to the correct rate calculated without the scaled quantities but using 1003/16 sources and the actual dimensions is

$$\left(\frac{\text{actual diameter}}{\text{scaled diameter}} \right)^{0.2} = \left(\frac{1003}{16} \right)^{0.1} \quad (2.7)$$

A factor of 0.5 over-prediction of the rate of condensation in the riser will be seen to be insignificant in Sections 5 and 6 because most of the condensation occurs before the slug enters the riser.

The principal inaccuracy is the assumption that all 1003 process tubes have the same temporal behavior. The fact that they don't have the same temporal behavior is a source of uncertainty in the analysis.

2.2. Fission Product Inventory

The fission product inventory in one process tube listed in Table 2.2 was calculated with the ORGEN2 computer code⁷ assuming 360.89 kg U^{238} and 3.65 kg U^{235} were exposed to 225 days at full power and 4.94 MW. The isotopes listed in the table represent most of the mass of the elements shown. Isotopic information is used only for the calculation of the effect of decay heat on the gas temperature so the inventories of several long-lived isotopes are combined to calculate a representative inventory of only one of the isotopes for each element.

Since the inventory is to be used in the next section to calculate a source rate for species, and since a satisfactory vapor phase chemistry model is not yet available to calculate the dynamic, coupled behavior of vapor chemical reactions and the effect of surface reactions or condensation of some of the reactants, a number of simplifying assumptions about the vapor chemistry are made. It is assumed that (1) all of the iodine released combines with cesium and that (2) cesium

TABLE 2.2. FISSION PRODUCT INVENTORY IN ONE PROCESS TUBE

Total Cesium 9.531 E-02 kg	
Cs 133	4.160 E-02 kg (4.367 E-01 fraction)
Cs 134	9.516 E-04 kg (9.989 E-03 fraction)
Cs 135	1.185 E-02 kg (1.244 E-01 fraction)
Cs 137	4.086 E-02 kg (4.289 E-01 fraction)
Cs 140	<u>1.700 E-07 kg</u> (1.785 E-06 fraction)
	9.526 E-02 kg
Total Iodine 9.780 E-03 kg	
I 129	8.343 E-03 kg (8.541 E-01 fraction) ²
I 131	1.089 E-03 kg (1.115 E-01 fraction)
I 132	1.893 E-05 kg (1.938 E-03 fraction)
I 133	2.440 E-04 kg (2.498 E-02 fraction)
I 135	7.295 E-05 kg (7.468 E-03 fraction)
I 137	<u>3.601 E-08 kg</u> (3.687 E-06 fraction)
	9.768 E-03 kg
Total Tellurium 1.737 E-02 kg	
Te 129M	2.124 E-04 kg (1.236 E-02 fraction)
Te 130	1.631 E-02 kg (9.491 E-01 fraction) ³
Te 131	2.110 E-06 kg (1.228 E-04 fraction)
Te 131M	2.488 E-05 kg (1.448 E-03 fraction)
Te 132	6.333 E-04 kg (3.685 E-02 fraction)
Te 133	1.427 E-06 kg (8.304 E-05 fraction)
Te 135	<u>2.735 E-08 kg</u> (1.596 E-06 fraction)
	1.718 E-02 kg
Total Krypton 1.308 E-02 kg	
Kr 85	1.306 E-02 kg (9.986 E-01 fraction) ⁴
Kr 85M	4.573 E-06 kg (3.497 E-04 fraction)
Kr 87	2.551 E-06 kg (1.951 E-04 fraction)
Kr 88	8.137 E-06 kg (6.222 E-04 fraction)
Kr 90	<u>3.180 E-08 kg</u> (2.432 E-06 fraction)
	1.308 E-02 kg
Total Xenon 1.756 E-01 kg	
Xe 133	1.756 E-01 kg (9.997 E-01 fraction) ⁵
Xe 133M	1.929 E-05 kg (1.098 E-04 fraction)
Xe 135	3.197 E-05 kg (1.820 E-04 fraction)
Xe 137	6.658 E-07 kg (3.791 E-06 fraction)
Xe 140	<u>1.991 E-08 kg</u> (1.134 E-07 fraction)
	1.756 E-01 kg

²I 127 and I 129 inventories were combined for fractional inputs to the analysis

³Te 122, 123, 124, 125, 126, 128, and 130 inventories were combined to calculate the fractional inputs to the analysis.

⁴Kr 80, 82, 83, 84, 86, and 85 inventories were combined to calculate the fractional inputs to the analysis.

⁵Xe 128, 130, 131, 132, 134, 136, and 133 inventories were combined to calculate the fractional inputs to the analysis.

not combined with iodine combines with steam to form cesium hydroxide. Thermochemical equilibrium calculations performed by Cronenberg^{8,9} for conditions present in tests with zircaloy and uranium dioxide^{8,9} have shown that these are reasonable assumptions as long as the temperature is not too high, the hydrogen-to-steam ratio is not too high, and the concentrations of cesium and iodine are not too low. For iodine and cesium concentrations of $6.12\text{E-}8$ kg-moles/m³ and $5.17\text{E-}7$ kg-moles/m³, respectively, Cronenberg finds CsI is the dominant form of iodine for temperatures up to at least 1700 K. He also finds CsOH is the dominant form of cesium for temperatures at least as high as 2000 K. These results are believed to be applicable to the N Reactor because boron compounds which react with cesium to shift the equilibrium distribution away from CsI¹⁰ are not present, and because there is no stainless steel in the hotter regions of the N Reactor to react with the CsOH and thus drive the

equilibrium to the right hand side by depleteing the CsOH.

It is also assumed (3) that tellurium will be released from the molten uranium as the element but will combine with any tin vapor (from zircaloy) to form tin telluride. Tellurium will react with both zirconium and tin⁹ but the vapor pressure of zirconium is so low at temperatures predicted for the N Reactor that it's presence in the vapor phase is negligible.

From the assumptions just made, the iodine is presumed to appear as

$$9.780\text{E-}03 \text{ kg I} * \frac{126.904 \text{ kg I/mole} + 132.905 \text{ kg Cs/mole}}{126.904 \text{ kg I/mole}} = 2.002\text{E-}02 \text{ kg CsI}$$

The cesium in excess of the amount present as cesium iodide is presumed to appear as

$$9.531\text{E-}02 \text{ kg Cs} - 2.002\text{E-}02 \text{ CsI} \frac{132.905 \text{ kg Cs/mole}}{126.904 \text{ kg I/mole} + 132.905 \text{ kg Cs/mole}} * \\ \frac{132.905 \text{ kg Cs/mole} + 15.9994 \text{ kg O/mole} + 1.00797 \text{ kg H/mole}}{132.905 \text{ kg Cs/mole}} =$$

$$9.595\text{E-}02 \text{ kg CsOH}$$

The inventory available for release is reduced by 1) a factor of one third since only a third of the length is modeled as a source (the end regions are considerably cooler) and by 2) a factor 0.318, the ratio of the volume of the inner fuel element to the total volume of fuel, because only the hotter inner annulus of uranium is assumed to fail and be exposed to the steam.

It will turn out that the calculated tellurium and tin source rates have such different temporal behavior that one must consider the release timing to calculate the species. This calculation will be explained in the next subsection.

2.3. Fission Products and Structural Materials

Table 2.3 shows the calculated fission product release rates from a process tube center section for the base case. The cesium iodide, cesium hydroxide, and tellurium are released from uranium fuel but the tin is released from Zircaloy cladding. The tin telluride release is determined from the intersection of the tellurium and tin release rates, as will be explained in Section 2.3.2.

2.3.1. Releases from Uranium Metal

The release rates from uranium metal were calculated using minor modifications of a model developed by K. R. Birney¹¹. This model assumes that the release of fission products from metallic uranium is proportional to the oxidation of the metal. For noble gases, iodine, and tellurium, the model specifies that complete oxidation of the metallic uranium releases 100% of the element. For cesium, the model provided by Reference 11 allows release of only 30% of the cesium based on observations from early experiments. For the base case, the release fractions at complete oxidation have been changed to 100% of the cesium and only 20% of the tellurium. The change in the cesium fraction was made because more recent experiments have shown that cesium reacts with silica in glass systems like the one used to determine the 30% fraction¹² so that the 30% detection was probably due to reactions after release rather than retention in the fuel matrix.

The change in the tellurium was made because the oxidation of the metallic fuel is not predicted to be complete and it is believed that the release of tellurium is not linear. It is apparently delayed until oxidation is nearly complete and the Te is no longer a minority species in the metal phase. The data in Figure 4 of Reference 11 suggest a slope corresponding to a total oxidation release fraction of about 0.2 until the metal is approximately 65% oxidized. A similar effect has been documented for tellurium and tin telluride release from oxidizing zircaloy metal¹³.

Oxidation rates of the metal were calculated using the expression

$$F = (1.35E-04 T_c - 0.123) t_m^{\frac{1}{2}} \quad (2.8)$$

where

$$\begin{aligned} F &= \text{fraction of uranium oxidized} \\ T_c &= \text{temperature } (^{\circ}\text{C}) \\ t_m &= \text{time at temperature (minutes),} \end{aligned}$$

provided in Reference 11 for oxidation of typical geometries (surface-to-volume ratios) of N-Reactor fuel. Equation (2.8) was converted to use temperature in Kelvin and time in seconds,

$$F = (1.74E-05 T - 0.0206) t^{\frac{1}{2}} \quad (2.9)$$

where

$$\begin{aligned} F &= \text{fraction of uranium oxidized} \\ T &= \text{temperature (K)} \\ t &= \text{time (s).} \end{aligned}$$

TABLE 2.3. CALCULATED FISSION PRODUCT AND STRUCTURAL MATERIALS RELEASE RATES FROM A PROCESS TUBE CENTER SECTION

Time (s)	CsI Release Rate (kg/s)	CsOH Release Rate (kg/s)
544.4	0.000E+00	0.000E+00
544.7	0.682E-05	0.327E-04
545.5	0.266E-05	0.127E-04
547.0	0.178E-05	0.855E-05
550.0	0.131E-05	0.628E-05
556.0	0.105E-05	0.503E-05
569.5	0.936E-06	0.448E-05
579.25	0.927E-06	0.444E-05
580.0	0.527E-06	0.252E-05
597.0	0.120E-06	0.573E-06
645.0	0.963E-07	0.462E-06
741.0	0.686E-07	0.329E-06
933.0	0.371E-07	0.178E-06

Time (s)	Te Release Rate (kg/s)	Sn Release Rate (kg/s)	SnTe Release Rate (kg/s)
544.4	0.000	0.000	0.000
544.7	1.183E-06	0.000	1.733E-10
545.5	4.606E-07	0.000	1.790E-10
547.0	3.095E-07	0.000	1.900E-10
550.0	2.274E-07	0.000	2.111E-10
556.0	1.821E-07	0.000	1.288E-10
569.5	1.622E-07	0.000	4.294E-10
579.25	1.605E-07	0.000	6.504E-10
580.0	9.105E-08	0.000	6.674E-10
580.75	2.162E-08	0.000	6.844E-10
597.0	2.019E-08	0.000	1.066E-09
645.0	1.362E-08	0.000	5.965E-09
697.8	0.000	0.000	2.702E-08
725.6	0.000	1.436E-08	2.446E-08
757.8	0.000	4.862E-08	2.205E-08
790.0	0.000	1.174E-07	2.028E-08

The next step in the application of Equation (2.9) is to generalize it to non-isothermal conditions. At any particular time Equation (2.9) implies a rate

$$\frac{dF}{dt} = \frac{1}{2} (1.74E-05 T - 0.0206) t^{-\frac{1}{2}} \quad (2.10)$$

It is important to write the rate equation in a form that contains those variables that physically control the rate before one inserts the time dependence of T and integrates. Equation (2.10) is only correct for the isothermal case. For other cases, one must replace t with something proportional to the reaction layer thickness because it is the reaction layer thickness instead of the time that controls the oxidation rate of a material like uranium which forms a protective oxide. (For example, two different T(t) histories can arrive at the same temperature and oxide thickness at different times. If temperature and oxide layer thickness are the controlling parameters, Equation (2.10) must be modified to predict the same rate at different times for these two histories.) From Equation (2.9)

$$t^{-\frac{1}{2}} = \frac{(1.74E-05 T - 0.0206)}{F} \quad (2.11)$$

and Equation (2.10) can be written

$$\frac{dF}{dt} = \frac{1}{2} \frac{(1.74E-05 T - 0.0206)^2}{F} \quad (2.12)$$

Equation (2.12) is in a form which contains the physically controlling variables. That is, the rate is expressed as a temperature-dependent term divided by a parameter that is proportional to the oxide thickness. One can incorporate the time dependence of T in this equation and integrate.

From the companion RELAP5 study, the temperature of the metal fuel (Heat Structure 0101100201) is

For t = 465 to 580 s

$$T = 1050 + \frac{(1370-1050)}{580 - 465} (t - 465) = 1050 + 2.7826(t - 465) \quad (2.13a)$$

and for t = 580 to 760 s

$$T = 1370 + \frac{(1385 - 1370)}{760 - 580} (t - 580) = 1370 + 0.083333(t - 580) \quad (2.13b)$$

Substitution of Equation (2.13) into Equation (2.12) and integration from the time the fuel cladding is presumed to fail (544.4 seconds, when the temperature is 1271 K¹⁴) yields the fraction of oxidation as a function of time. Table 2.4 shows the calculated fraction as a function of time

TABLE 2.4. FRACTION OF URANIUM OXIDIZED

Temperature (K)	Time (s)	Fraction _____	Average Time (s)	<u>(s⁻¹)</u>
1271.0	544.4	0.000		
			544.7	3.213E-03
1272.6	545.0	1.928E-03		
			545.5	1.251E-03
1275.4	546.0	3.179E-03		
			547.0	8.408E-04
1281.0	548.0	4.861E-03		
			550.0	6.178E-04
1292.1	552.0	7.332E-03		
			556.0	4.947E-04
1314.3	560.0	1.129E-02		
			569.5	4.409E-04
1367.2	579.0	1.967E-02		
			579.25	4.367E-04
1368.6	579.5	1.988E-02		
			580.0	2.482E-04
1370.0	580.5	2.013E-02		
			580.75	5.965E-05
1370.1	581.0	2.016E-02		
			597.0	5.631E-05
1372.7	613.0	2.193E-02		
			645.0	4.540E-05
1378.1	677.0	2.484E-02		
			741.0	3.231E-05
1388.7	805.0	2.898E-02		
			933.0	1.747E-05
1410.1	1061.0	3.345E-02		

and temperature. It is interesting to note that the calculated fraction is only 0.033 at 1061 seconds. The differential method that was used to find average oxidation rates for the time increments shown is apparent from an inspection of the table and the release rate in fraction of the inventory per second versus time is illustrated in Figure 2.2. The decrease in the rate at 580 s corresponds to the change in heating rate that occurs at this time. (One of the reviewers, D. A. Petti, has correctly pointed out that use of Equation (2.12) directly instead of an interpolation approach would have been more appropriate. The author agrees but does not feel the difference is significant enough to require a repeat of the calculations with this change.)

2.3.2. Release Rates from Zircaloy Cladding

The mechanism for release of tin is quite different than that for the other species discussed. Release rates of tin were calculated using a model developed for the SCDAP/RELAP5 computer code¹⁵. The rate of mass transport from the cladding surface is presumed to be proportional to the surface area, A_w ; the mass-transport coefficient for transfer between bulk gas flow and the wall surface-gas interface, k_w ; and the difference between the concentration of tin in the gas phase and it's equilibrium concentration, $C - C_{eq}$:

$$\frac{dM}{dt} = -A_w k_w (C - C_{eq}) \quad (2.14)$$

It is assumed that $C \ll C_{eq}$ and that the mass transport coefficient used by TRAP-MELT²² (a modified Dittus-Boelter heat transfer coefficient) is appropriate. Thus

$$\frac{dM}{dt} \approx -A_w \frac{0.023 \text{ Re}^{0.83} \text{ Sc}^{0.33} D_v}{D_{ia}} C_{eq} \quad (2.15)$$

where

Re = Reynold's Number, density speed D_{ia} / viscosity
 Sc = Schmidt Number, viscosity / (density D_v)
 D_v = diffusivity of Tin vapor in steam (m^2/s)
 and D_{ia} = diameter of the pipe (m)

For the N Reactor the Reynold's number is approximately 29,500, the Schmidt number is approximately 0.486, the diffusivity of the tin vapor is approximately $2.06 \text{ E-}04 \text{ m}^2/\text{s}$, and the effective diameter of the first volume modeled is approximately $3 \text{ E-}02 \text{ m}$ so the mass transfer coefficient is approximately 0.65 m/s .

The equilibrium vapor pressure was calculated by multiplying the equilibrium tin vapor concentration correlation¹⁶

$$C_{eq} = \frac{118.69}{8.31 \text{ E}+03 T_{wall}} \exp \left\{ \frac{-2.847 \text{ E}+04}{T_{wall}} + 4.548 \ln(T_{wall}) - 14.31 \right\} \quad (2.16)$$

times the mole fraction of tin in Zircaloy, 0.012, as required by Raoult's

Figure 2.2. Fractional release rate of fission products inventories from fuel exposed to steam at 544.4 s.

law. Since only a small fraction of the tin was released, it was not necessary to correct the fraction for the amount of tin released.

Table 2.5 lists the time, Zircaloy temperature, and tin release rates calculated by the method just described and Table 2.6 lists the rate of release of tellurium calculated with the method of Section 2.3.1. The revised rates in each of these tables are the initial rates minus the mass lost to the reaction

which is assumed to go to completion and consume all of the minority species. Table 2.7 is a listing of the basic computer codes that were used to correct the tin and tellurium release rates at a given time by interpolating the companion table's release rates, correcting for the molar weight difference of the two elements and printing the amount of tin telluride production that results from the reaction.

2.4. Aerosol Sources

It is difficult to identify a significant source of aerosols within the pressure tubes of the N Reactor. It turns out, partly because the burnup is limited and partly because the surface-to-volume ratio is large, that none of the fission products release rates calculated in Section 2.3.1 are sufficient to exceed saturation. The same is true for the rate of release of tin from the Zircaloy cladding. Another potential source of aerosol is the evaporation of volatile metals followed by oxidation to compounds with much lower vapor pressures. However, both Zircaloy and uranium metals, the obvious candidates, have vapor pressures that are so low that they are not significantly different from the oxides. Yet another potential source of aerosols, boron compounds from the coolant, are not present in the N-Reactor. Rapid cooling of the vapor to temperatures below saturation is not a viable mechanism because the cooling is by heat transport from hot gas to cooler walls. In this situation, condensable species transport to the wall as fast as heat does so concentrations decrease along with the gas temperature.

It has been suggested that a mechanical aerosol could be formed by Zircaloy undergoing oxidation.¹⁷ However, none of the separate effects studies of Zircaloy oxidation^{17,18} has ever reported a mechanical aerosol. The cladding oxide has always been characterized as an adherent, protective oxide.

On the other hand, it is difficult to assume that there is absolutely no source of a "seed" for an aerosol. Impurities such as minor amounts of dissolved silicon in the coolant water are one potential source, and corrosion products are another. For this reason the base case was run with a fairly low concentration, the threshold limit for nuisance dusts reported on page 10 of Hinds¹⁹ which is 10 mg/m^3 or approximately 1.0 E-07 kg/s with the steam source rates predicted for the N Reactor transient. Zircaloy dioxide was selected as a representative low volatile species. The geometric mean particle volume of 1.7 E-18 m^3 and geometric standard deviation based on volume of 6 are characteristic of the MnO aerosol used in the LACE LA-1 experiment⁴.

TABLE 2.5. TIN RELEASE RATE CALCULATION RESULTS

<u>Time</u> <u>(s)</u>	<u>Temperature</u> <u>(K)</u>	<u>Tin Release Rate</u> <u>(kg/s)</u>	<u>Revised Tin Release</u> <u>(kg/s)</u>	<u>SnTe Release</u> <u>(kg/s)</u>
500.0	950	9.559E-12	0.000	
532.2	1000	4.054E-11	0.000	
564.4	1050	1.512E-10	0.000	
596.7	1100	5.041E-10	0.000	
628.9	1150	1.524E-09	0.000	
661.1	1200	4.225E-09	0.000	
693.3	1250	1.087E-08	0.000	
725.6	1300	2.615E-08	1.436E-08	2.446E-08
757.8	1350	5.924E-08	4.862E-08	2.205E-08
790.0	1400	1.272E-07	1.174E-07	2.028E-08

TABLE 2.6. TELLURIUM RELEASE RATE CALCULATION RESULTS

<u>Time</u> <u>(s)</u>	<u>Te Release Rate</u> <u>(kg/s)</u>	<u>Revised Te Release</u> <u>(kg/s)</u>	<u>SnTe Release</u> <u>(kg/s)</u>
544.4	0.000	0.000	0.000
544.7	1.183E-06	1.183E-06	1.733E-10
545.5	4.607E-07	4.606E-07	1.790E-10
547.0	3.096E-07	3.095E-07	1.896E-10
550.0	2.275E-07	2.274E-07	2.111E-10
556.0	1.822E-07	1.821E-07	1.288E-10
569.5	1.624E-07	1.622E-07	4.294E-10
579.25	1.608E-07	1.605E-07	6.504E-10
580.0	9.140E-08	9.105E-08	6.674E-10
580.75	2.197E-08	2.162E-08	6.844E-10
597.0	2.074E-08	2.019E-08	1.066E-09
645.0	1.672E-08	1.363E-08	5.965E-09
741.0	1.190E-08	0.000	
933.0	6.433E-09	0.000	

TABLE 2.7. COMPUTER CODES USED TO CORRECT TIN AND TELLURIUM RELEASES

```

10 REM snte2.bas
20 REM program to calculate snte source rate from sn and te rates
30 REM part one correct sn rate
40 INPUT "please enter time . sn source rate ":T,SNRATE
50 PRINT "time = ",T,"tin rate = ",SNRATE
60 INPUT "please enter earlier te time, te rate for interpolation ":TME,TEE
70 INPUT "please enter later te time, te rate for interpolation ":TML,TEL
80 PRINT "times, tellurium source rates interpolated follow"
90 PRINT TME,TEE,"      ",TML,TEL
100 TERATE = TEE + (TEL - TEE) * (T - TME) / (TML - TME)
110 SNRATE = SNRATE - TERATE * 118.69 / 127.6
120 SNTER = TERATE * (127.6 + 118.69) / 127.6
121 PRINT "revised sn rate = ",SNRATE,"snte rate = ",SNTER
130 GOTO 40

```

```

10 REM snte.bas
20 REM program to calculate snte source rate from sn and te rates
30 REM part one correct te rate
40 INPUT "please enter time . te source rate ":T,TERATE
50 PRINT "time = ",T,"tellurium rate = ",TERATE
60 INPUT "please enter earlier sn time, sn rate for interpolation ":TME,SNE
70 INPUT "please enter later sn time, sn rate for interpolation ":TML,SNL
80 PRINT "times, tin source rates interpolated follow"
90 PRINT TME,SNE,"      ",TML,SNL
100 SNRATE = SNE + (SNL - SNE) * (T - TME) / (TML - TME)
110 TERATE = TERATE - SNRATE * 127.6 / 118.69
120 SNTER = SNRATE * (127.6 + 118.69) / 118.69
121 PRINT "revised te rate = ",TERATE,"snte rate = ",SNTER
130 GOTO 40

```

2.5. Wall Temperatures and Initial Gas Temperature

Wall temperatures for the five volumes are listed in Table 2.8. The temperatures for the fueled part of the process tube and the riser were taken from the companion RELAP5 analysis but those of the spacer part of the process tube were taken from a supplemental analysis by S. Wagoner⁵ (included as Appendix A) that was carried out because it was believed that the RELAP5 analysis temperatures were too high due to lack of a surface heat structure in the first analysis. Temperatures at times not listed in the table were interpolated by the fission product behavior analysis tool.

Initial gas temperatures were taken from the companion RELAP5 analysis. They were linearly interpolated from 1000 K at 500 s to 1350 K at 750 s. The initial gas temperature is not an important parameter because the surface-to-volume ratio of the N Reactor is large and the resultant high heat transfer causes the gas temperature to approach the wall temperature rapidly.

2.6. Steam Flow rates

Steam flow rates were 1.14 E-02 kg/s for times less than 550 s, linearly interpolated from 1.14 E-02 at 550 s to 7.42 E-03 kg/s at 600 s, and 7.42 E-04 kg/s for times greater than 600 s. These rates were obtained from the supplemental analysis by S. Wagoner⁵ that was used for wall temperatures. The flow rates are an average of the flow rates Wagoner found for levels 1, 2, 3, 6, and 8 of the process tubes. The variation from level-to-level is less than the flow rate changes tested and discussed in Section 6.3. These rates correspond to a velocity of approximately 50 m/s in the fueled part of the process tubes and 20 m/s in the connectors.

2.7. Input to the Analysis Tool

A list of the input requirements for the analysis tool used to study fission product behavior in the N Reactor is provided in Appendix B. It is included to assist the reader in understanding Table 2.9 which is a copy of the input data used for the best-estimate case in this analysis.

TABLE 2.8. WALL TEMPERATURES USED IN THE ANALYSIS

Time	Volume:	1	2	3	4	5
		<u>Center 1/3</u> <u>Process Tube</u>	<u>End 1/3</u> <u>Process Tube</u>	<u>Spacers</u>	<u>Connector</u> <u>Tube</u>	<u>Standpipe</u>
500 s		950 K	880 K	507 K	-	-
534 s		-	-	-	-	484 K
620 s		-	1010 K	-	-	-
635 s		-	-	-	485 K	-
700 s		-	-	583 K	507 K	486 K
790 s		1400 K	-	-	-	-

TABLE 2.9. LIST OF INPUT DATA USED IN THE BASE CASE

NUMBER OF VOLUMES = 5									
NUMBER OF SUBVOLUMES = 2 2 5 2 8 4									
VOLUME	LENGTH	CROSS SECTION AREA	WALL SURFACE	SETTLING SURFACE	AREA	WALL TYPE			
1	.3539E+01	.6836E-C3	.8415E+00	.2679E+00		0			
2	.3233E+01	.6836E-C3	.8415E+00	.2679E+00		0			
3	.3797E+01	.3214E-C2	.8105E+00	.2560E+00		0			
4	.1680E+02	.2113E-C2	.2822E+01	.8982E+00		1			
5	.7147E+01	.2005E-C2	.1085E+00	.2005E+00		1			
VOLUME NUMBER 1 PIPE BEND RADII IN EACH SUBVOLUME									
	.000E+00	.000E+00							
VOLUME NUMBER 2 PIPE BEND RADII IN EACH SUBVOLUME									
	.000E+00	.000E+00							
VOLUME NUMBER 3 PIPE BEND RADII IN EACH SUBVOLUME									
	.000E+00	.157E+01							
VOLUME NUMBER 4 PIPE BEND RADII IN EACH SUBVOLUME									
	.157E+01	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.157E+01	
VOLUME NUMBER 5 PIPE BEND RADII IN EACH SUBVOLUME									
	.000E+00	.000E+00	.000E+00	.000E+00					
INITIAL TIME = .544E+03 FINAL TIME = .600E+03									

TABLE 2.9 LIST OF INPUT DATA USED IN THE BASE CASE (CONTINUED)

SPECIES CONSIDERED I2 1 CSI CSFH T5 0 C3 AG 0 SRDH2 BADH2 H2TE HI 1 SN 1 SNTF 1 H2O 1 ZRO2 0 UO2 0 C 0 XX 0 YY 0 YX 0

TOLERANCE 1 1.00E+00 TOLERANCE 2 1.00E-06

PRINT FREQUENCY CONTROL = 1 PRINT AMOUNT CONTROL = 6

CESIUM ISOTOPE FRACTIONS20
FR(133) = .438E+00 FR(134) = .999E-02 FR(135) = .124E+00 FR(137) = .429E+00 FR(140) = .179E-05

IODINE ISOTOPE FRACTIONS20
FR(127) = .854E+00 FR(131) = .112E+00 FR(132) = .194E-02 FR(133) = .250E-01 FR(135) = .747E-02 FR(137) = .369E-05

KRYPTON ISOTOPE FRACTIONS20
FR(83) = .999E+00 FR(85M) = .350E-03 FR(87) = .195E-03 FR(86) = .622E-03 FR(90) = .243E-05

TELLURIUM ISOTOPE FRACTIONS20
FR(128) = .124E-01 FR(130) = .949E+00 FR(131) = .123E-03 FR(131M) = .145E-02 FR(132) = .369E-01 FR(133) = .830E-04 FR(135) = .160E-05

XENON ISOTOPE FRACTIONS20
FR(133) = .100E+01 FR(135M) = .110E-03 FR(135) = .132E-03 FR(137) = .379E-05 FR(140) = .113E-06

SOURCE RATE TABLE FOR CSI VAPOR TIME (S) MASS RATE (KG/S) PAIRS		
NUMBER OF PAIRS	14	
.5444E+03	.0000E+00	
.5447E+03	.6818E-05	
.5455E+03	.2655E-05	
.5470E+03	.1784E-05	
.5500E+03	.1311E-05	
.5560E+03	.1050E-05	
.5699E+03	.9355E-06	
.5793E+03	.9267E-06	
.5800E+03	.5267E-06	
.5808E+03	.1266E-06	
.5970E+03	.1195E-06	
.6450E+03	.9634E-07	
.7410E+03	.6857E-07	
.9330E+03	.3707E-07	

AEROSOL TYPE SWITCH = 2

SOURCE RATE TABLE FOR CSFH VAPOR TIME (S) MASS RATE (KG/S) PAIRS		
NUMBER OF PAIRS	14	
.5444E+03	.0000E+00	
.5447E+03	.3266E-04	
.5455E+03	.1272E-04	
.5470E+03	.8555E-05	
.5500E+03	.6283E-05	
.5560E+03	.5031E-05	
.5699E+03	.4484E-05	
.5793E+03	.4482E-05	
.5800E+03	.2342E-05	
.5808E+03	.6067E-06	
.5970E+03	.5727E-06	
.6450E+03	.4617E-06	
.7410E+03	.3286E-06	
.9330E+03	.1777E-06	

AEROSOL TYPE SWITCH = 2

TABLE 2.9 LIST OF INPUT DATA USED IN THE BASE CASE (CONTINUED)

SOURCE RATE TABLE FOR		TE VAPOR TIME (S)	MASS RATE (KG/S)	PAIRS
NUMBER OF	PAIRS			
	13			
	.5444E+03	.333CE+00		
	.5447E+03	.1183E-05		
	.5455E+03	.4606E-06		
	.5470E+03	.333CE+00		
	.5500E+03	.2274E-06		
	.5500E+03	.1821E-06		
	.5693E+03	.1821E-06		
	.5793E+03	.1603E-06		
	.5800E+03	.9103E-07		
	.5808E+03	.2102E-07		
	.5970E+03	.2015E-07		
	.6450E+03	.1305E-07		
	.6978E+03	.300CE+00		

AERCSOL TYPE SWITCH = 2

SOURCE RATE TABLE FOR		SN VAPOR TIME (S)	MASS RATE (KG/S)	PAIRS
NUMBER OF	PAIRS			
	4			
	.5978E+03	.300CE+00		
	.7236E+03	.1436E-07		
	.7578E+03	.4062E-07		
	.7950E+03	.1174E-06		

AERCSOL TYPE SWITCH = 2

SOURCE RATE TABLE FOR		STE VAPOR TIME (S)	MASS RATE (KG/S)	PAIRS
NUMBER OF	PAIRS			
	16			
	.5444E+03	.000CE+00		
	.5447E+03	.1733E-09		
	.5455E+03	.179CE-09		
	.5470E+03	.1897E-09		
	.5500E+03	.2111E-09		
	.5500E+03	.1258E-09		
	.5693E+03	.4294E-09		
	.5793E+03	.6504E-09		
	.5800E+03	.8074E-09		
	.5808E+03	.6844E-09		
	.5970E+03	.1056E-08		
	.6450E+03	.3565E-08		
	.6978E+03	.3702E-07		
	.7236E+03	.3446E-07		
	.7578E+03	.2205E-07		

.7900E+03 .2026E-07

AERCSOL TYPE SWITCH = 2

SOURCE RATE TABLE FOR		H2O VAPOR TIME (S)	MASS RATE (KG/S)	PAIRS
NUMBER OF	PAIRS			
	2			
	.5000E+03	.114CE-01		
	.500CE+03	.7422E-02		

AERCSOL TYPE SWITCH = 2

TABLE 2.9 LIST OF INPUT DATA USED IN THE BASE CASE (CONTINUED)

SOURCE RATE TABLE FOR ZPC2VAPOR		TIME (S)	MASS RATE (KG/S)	PAIRS
NUMBER OF PAIRS	=	8		
.5000E+03		.7935E-33		
.5357E+03		.4734E-31		
.5714E+03		.2921E-29		
.6071E+03		.1553E-28		
.6429E+03		.194E-26		
.6786E+03		.1976E-25		
.7143E+03		.2595E-24		
.7500E+03		.2772E-23		

AEROSOL TYPE SWITCH = 0

NUMBER OF AEROSOL TIME PAIRS 1

SOURCE RATE TABLE FOR ZR02 AEROSOL

TIME, XBAR, SIG AND RMASS TABLE

.500E+03 .166E-17 .600E+01 .422E-06

TIME = .500E+03

.131E-20	.138E-22	.520E-19	.700E-16	.337E-13	.580E-11	.356E-09	.782E-08	.613E-17	.172E-06
.174E-06	.615E-07	.785E-08	.358E-09	.584E-11	.340E-13	.708E-16	.126E-19	.140E-32	.000E+00

SOURCE RATE TABLE FOR GAS

TIME (S)	MASS RATE (KG/S)	HE	AR	KR	XE	H2	N2	O2	CO	CD2	H2O	MOLE FRACTIONS
NUMBER OF ENTRIES = 1	.544E+03	.100E-11	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00	.000E+00

TABLE 2.9 LIST OF INPUT DATA USED IN THE BASE CASE (CONTINUED)

INITIAL BULK GAS TEMPERATURE - TIME(S) TEMPERATURE(K)			
NUMBER OF ENTRIES =	2		
	.2000E+03	.1000E+04	
	.7500E+03	.1350E+04	
WALL SURFACE TEMPERATURES - TIME(S) TEMPERATURE(K)			
VOLUME NUMBER =	1		
	.5000E+03	.9500E+03	
	.7500E+03	.1400E+04	
VOLUME NUMBER =	2		
	.2000E+03	.8800E+03	
	.6000E+03	.1010E+04	
VOLUME NUMBER =	3		
	.5000E+03	.5070E+03	
	.7500E+03	.5830E+03	
VOLUME NUMBER =	4		
	.6500E+03	.4850E+03	
	.7000E+03	.5070E+03	
VOLUME NUMBER =	5		
	.3340E+03	.4830E+03	
	.7000E+03	.4860E+03	
GAS INPUT PRESSURE - TIME(S) PRESSURE(PA)			
NUMBER OF ENTRIES =	2		
	.2000E+03	.1000E+06	
	.6000E+03	.1000E+06	
BOUNDARY CONDITIONS TIME CONSTANT - TIME(S) TIME CONSTANT(S)			
NUMBER OF ENTRIES =	12		
	.2444E+03	.2000E+00	
	.3450E+03	.1000E+01	
	.3470E+03	.2000E+01	
	.3550E+03	.4000E+01	
	.5750E+03	.4000E+01	
	.5740E+03	.2000E+01	
	.5700E+03	.1000E+01	
	.5700E+03	.3000E+00	
	.5710E+03	.1000E+01	
	.5720E+03	.1000E+01	
	.5660E+03	.1000E+01	
	.5950E+03	.4000E+02	
DEBUG SWITCH =	ALL		

3. TESTING OF THE ANALYSIS TOOL

The analysis tool used in this study employs the fission product transport models of TRAP-MELT2.0 but has been completely recoded. The Lagrangian or slug flow formulation was used in place of the traditional Eulerian or control volume approach because the well-mixed assumption of Eulerian formulations is not efficient for the long channels of the N Reactor. Because the coding of the aerosol behavior models had not been tested against aerosol transport data, and because a new model for aerosol deposition at pipe bends was added, the tool was tested against the pipe data of the LACE LA-1 test⁴.

The results with and without the pipe bend model are compared to the data and the TRAP-MELT predictions by Battelle Columbus Laboratories in Figure 3.1. The figure shows that the Lagrangian model duplicates the TRAP-MELT results when the pipe bend model is not added to the Lagrangian model and over-predicts the measured deposition rate even more when the pipe bend model is included. Inspection of these results has yielded three relevant conclusions:

- 1) The benchmark against LA1 is really a test of only one model, the inertial aerosol impaction model of TRAP-MELT2, because this mechanism dominates the others (as discussed below),
- 2) The over-prediction of the data is probably due to the lack of an aerosol resuspension model which one would expect to be important at the high velocities ($\approx 100\text{m/s}$) and high aerosol source rates ($6.5\text{E-}04\text{ kg/s MnO}$ and $4.8\text{E-}04\text{ kg/s CsOH}$ into 0.160 kg/s steam plus $0.190\text{ kg/s nitrogen}$) used in the LA1 test, and
- 3) Even with the aerosol resuspension observed in the LA1 test, substantial amounts of aerosol were removed from the flow stream. The main effect of resuspension was to delay the removal until discontinuities in the wall surface were encountered.

One can see that the inertial impaction model is dominant by calculating the aerosol deposition rate with just this model. The model provides a deposition velocity which is used in an expression of the form

$$C(t) = C(0) \exp\left(-\frac{v_{\text{dep}} A}{V} t\right) \quad (3.1)$$

where

$C(t)$ = the aerosol concentration at time t (kg/m^3)
 v_{dep} = the deposition velocity (m/s)
 A = the surface area (m^2)
 V = the volume (m^3).

The area-to-volume ratio of the pipe is $2/\text{radius} = 2/0.315\text{ m}$ for LA1.

For the fluid velocities of the LA1 experiment, the inertial impaction deposition velocity is calculated with the correlation

Figure 3.1. LA1 Pipe test comparison.

$$V_{dep} = \left\{ \begin{array}{l} \text{the lesser of 0.1 and} \\ \sqrt{0.0014 + \frac{0.125}{Re^{0.32}}} + 2E-8Re \end{array} \right\} \sqrt{0.0014 + \frac{0.125}{Re^{0.32}}} V_{fluid} \quad (3.2)$$

where

Re = Reynold's number (unitless)
 V_{fluid} = fluid velocity (m/s)

For the LA1 Reynold's number of 317,800, the deposition velocity is approximately 0.4 m/s. This velocity implies a characteristic time of

$$\tau = \frac{V}{A V_{dep}} = 0.04 \text{ s} \quad (3.3)$$

in Equation (3.1) which, in turn, implies a characteristic length of about four meters at a fluid velocity of about 100 m/s. Therefore, this model predicts that $1 - \exp(-1) \approx 0.63$ of the input aerosol is deposited in the first four meters of the pipe, and 0.63 of the remaining aerosol is deposited in the next four meters of pipe, etc. The model alone produces the result shown in Figure 3.1 and the other contributions to the aerosol deposition are negligible.

The conclusion that the over-prediction of the data is probably due to the lack of an aerosol resuspension model is largely based on visual inspection of the LA1 test pipe¹⁷. This inspection showed accumulation of aerosols at discontinuities in the pipe's internal structure and material that looked as though it had been transported along the pipe wall instead of in the aerosol.

The conclusion is indirectly supported by data from the Power Burst Facility Severe Fuel Damage Scoping Test¹⁸ and Test 1-1¹⁹ at velocities on the order of 10 and 1 m/s. In these tests, radioactive material was concentrated at the pipe bends and restrictions as the analysis models predict. The presence of greater concentrations at the pipe bends in the lower-velocity experiments and their absence in the higher-velocity experiments suggests that the material deposited at the bends in both experiments but was removed by resuspension in the higher-velocity LA1 experiment.

Before proceeding to discuss differences between the LA1 experiment and the cold leg break problem under consideration, it is worth noting from Figure 3.1 that the data do show eventual deposition of most of the aerosol. If one assumes that resuspension is the reason the model over-predicts the amount of material found in the upstream sections of the LA1 pipe, one should also conclude that most of the resuspended aerosol eventually finds a favorable site for deposition. The conclusion suggests that an appropriate approach to resuspension modeling might be to start with the concept of trapping sites that hold limited amounts of deposited aerosols.

Table 3.1 is a comparison of key parameters for the LA1 experiment with the corresponding parameters of the cold leg break analysis. The table shows that while the pipe diameters are similar and the coolant flow rates are similar in the fueled part of the process tubes, the coolant flow rates in the spacers and downstream volumes is more similar to the PBF tests where resuspension was not so pronounced. This suggests that aerosol deposition in the fueled part of the process tubes may be over-predicted by the turbulent deposition and pipe bend models but it may not be over-predicted in the spacer and downstream volumes. The pipe bend model was removed from the base case run because of the over-prediction of the LA1 data but the velocity differences and the great difference in aerosol source rates means that a net over-prediction is not certain so some analysis was done with the pipe bend model.

A major difference between the LA1 experiment and the cold leg break analysis shown in Table 3.1 is the temperatures. In the cold leg break, temperatures in the process tube are much higher than the 520 K used for the LA1 experiment. An examination of several species' equilibrium vapor concentrations calculated by the analysis tool versus temperature and given in Figures 3.2 and 3.3, indicates that these temperature differences imply that saturation concentrations in the cold leg break analysis will be orders of magnitude higher than they were in the LA1 experiment. There are also larger temperature decreases in the wall temperature as one proceeds downstream in the cold leg break analysis. This means that heat and vapor transport from the fluid (and any aerosol in it) to the wall will be more significant in the cold leg break analysis than it was during the LA1 experiment.

These differences will have considerable affect on the transport of fission products as an aerosol. The high process tube temperatures of the cold leg break analysis prevent formation of aerosols of cesium iodide, cesium hydroxide, or tellurium and delay condensation onto any pre-existing "seed" of low-volatile material until after the gas has cooled. Because the walls are a sink for both thermal energy and vapor, conditions in the cold leg break analysis may cause most of the vapor to condense on walls before the gas cools sufficiently to start condensation on aerosols or there may be a rapid condensation onto any pre-existing aerosol that is transported with the gas as it cools. The initial distribution between aerosols and walls will be dependent of the details of timing and concentration. Also, any aerosol with fission products formed during the cold leg break will experience revaporization from the aerosol because of the decreasing wall temperatures in the downstream volumes which maintain a temperature gradient between the gas and the walls.

In the LACE experiment, the small temperature differences and high aerosol concentrations encouraged initial condensation on both aerosols and walls. Additional vapor transport to downstream walls was not significant because the wall temperatures were nearly constant over the length of the pipe used in the experiment.

TABLE 3.1. COMPARISON OF PARAMETERS FOR LA1 AND COLD LEG BREAK

	LA1	COLD LEG BREAK
Pipe Inlet Temperature (K)	520	1000 - 1350
Walls Temperatures (K)	519	950 - 1400 880 - 1010 507 - 583 485 - 507
	510	484 - 486
Pipe Diameter (m)	0.063	0.030
Source Rates (kg/s)		
N ₂	0.190	0
H ₂ O	0.160	8.5 E-04 - 5.1 E-04
CsOH Vapor	6.0 E-09	0
MnO (ZrO ₂) Vapor	3.5 E-12	0
CsOH Aerosol	4.8 E-04	0 → 0.327 E-04 → less ⁶
MnO (ZrO ₂) Aerosol	6.5 E-04	0
CsI	0	0 → 0.682 E-05 → less
Te	0	0 → 0.118 E-05 → less
Sn	0	0 → 0.117 E-06
SnTe	0	0 → 0.270 E-07
Velocity (m/s)	96	70 (fueled process tubes) 20 (connectors)

⁶The word less is added to remind the reader that the release of fission product species in the cold leg break analysis is at the maximum rate for only a very short time. Figure 2.2 illustrates the time dependence of the release.

Figure 3.2. Equilibrium Vapor Concentrations versus temperature.

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Figure 3.3. Equilibrium Vapor Concentrations versus temperature.

4. MODIFICATIONS TO THE ANALYSIS TOOL TO STUDY THE N-REACTOR

The analysis tool used in this scoping study was developed to analyze fission product transport in the fission product sampling line of the Power Burst Reactor at the Idaho National Engineering Laboratory. Because this line was a single tube with no parallel connection and the N-Reactor process tubes contain three parallel channels, it was necessary to modify the approach of the analysis tool or to try to scale some volumes appropriately. Scaling of the process tubes was ruled out because it was expected that questions of evaporation/condensation of aerosols (or onto aerosols) would be important and non-linear effects make it difficult to scale correctly for all of the aerosol behavior phenomena. On the other hand, scaling of all of the volumes downstream was ruled out because it became clear after the first results were available that much of the vapor condensation would occur in the spacer and connector volumes. While the wall surface of the downstream volumes could be scaled to compensate for the fact that the inner annulus flow but not the by-pass flow is considered, scaling can not be done to correct both the wall surface area and the concentration in the expression for the condensation rate,

$$\frac{dC}{dt} = - \frac{A_w k_w}{V} [C - C_{eq}] \quad (4.1)$$

where

C = vapor concentration (kg of vapor/m³)
 C_{eq} = equilibrium vapor concentration at the wall temperature (kg/m³)
 A_w = wall surface area available to the slug (m²)
 k_w = mass transport coefficient for transfer between bulk gas flow and the wall surface - gas interface (m/s)
 V = slug volume (m³)

For this scoping study, it was decided to maintain the approach of modeling the fission product behavior in a single slug of fluid proceeding down a series of volumes. Scaling geometries in the process tube or the connector tube was avoided by treating the flow in the outer channel and inner circular channel as a by-pass flow that did not receive fission products until it returned to the main stream carried by the inner annulus at the spacer region.

The analysis tool was modified to assume that the fluid sources in the first volume were really 0.4223 (the ratio of the cross-sectional area of the inner annulus channel to the total cross-sectional area of all three channels) of the steam flow that entered the process tube. Hydrogen in the first volume is assumed to have been produced by a reaction

where M is either zirconium or uranium. Thus (1 - 0.4223) moles of steam are allowed to rejoin the gas slug at the spacer for every 0.4223 mole of hydrogen in the slug.

All of the modifications to the analysis code for the N Reactor analysis are contained in a separate update section labeled *IDENT DXHNRTR. They

include not only the bypass channel addition discussed in this section but also removal of the pipe bend model for some cases.

5. BEST ESTIMATE RESULTS

The base-case or best estimate analysis considers times from 544 to 600 s, the time span during which most of the fission product release was calculated to occur. Appendix A contains a microfiche of the detailed analysis results for this case and the input data that were discussed in Section 2. A sensitivity study of the effect of changes to the input are discussed in Section 6. The following sections are a discussion of the behavior calculated for the aerosol and the behavior of the fission product species in the best estimate problem. Time constants are used to guide the discussion in both sections.

Tables 5.1 to 5.5 show the calculated spacial distribution and states of cesium iodide (CsI), cesium hydroxide (CsOH), tellurium (Te), tin telluride (SnTe), and zirconium dioxide (ZrO₂) at 600 s. The distribution of steam/water is not presented in a table because the steam did not condense and the distribution of tin is not shown because the release rate of tellurium is greater than that of tin over the 544 to 600 time span so all of the released tin reacts with tellurium to form tin telluride. For cesium iodide, cesium hydroxide, and tellurium, 2.1 E-02 of the inventory in the hot-node uranium has been released. This is only 2.3 E-03 of the process tube inventory. Because of the very low concentration of these species and the high calculated wall temperatures of the process tubes, condensation of these species does not occur until the spacers, where the calculated wall temperatures are 507 to 583 K. Most of the very low volatility aerosol (ZrO₂) that was assumed to exist deposits in the process tube but some of the smaller particles are carried downstream. These results are discussed in more detail in the remainder of this section.

5.1. Aerosol Behavior

Inspection of the detailed print-out of Appendix A shows that cesium iodide, cesium hydroxide, tellurium, and tin telluride do not exceed their saturation concentrations in the center of the process tube, even during the rapid UO₂ oxidation and fission product release that occurs when uranium is first exposed to steam at 544.5 s. For this reason these species will neither form an aerosol nor condense on any pre-existing aerosol.

The behavior of the ZrO₂ aerosol that was presumed to be generated in the hot regions of the process tube is not unlike the behavior calculated for the LA1 pipe test at the start of the cold leg break analysis when fluid speeds are high. In the N-Reactor, the time constant for the geometric mean particle size to deposit in the center 1/3 is 1.4E-02 s, a number that implies a characteristic length of the order of only 0.95 meter for deposition of the geometric mean particle volume at the initial fluid speed of 68 m/s. The time constant is shorter for larger particles and longer for smaller ones. In the connector tubes, where the fluid speed is 31 m/s at the start of the analysis, the time constant for the geometric mean particle size is 1.3 s and the characteristic length is 39 meters, about twice the length of the volume. If, as was the case in the LACE LA1 test, the model is over-predicting the rate of aerosol deposition by a factor of two or three in the volumes where fluid flow is $\approx 100\text{m/s}$, more of the aerosol would be transported downstream to the

TABLE 5.1. CALCULATED CsI DISTRIBUTION AT 600 SECONDS

Mass released from uranium	4.57 E-05 kg
Mass chemisorbed	0
Mass condensed	4.56 E-05 kg
Mass deposited as aerosol	8.84 E-09 kg

Volume	Mass Condensed (kg)	Mass Deposited as Aerosol (kg)
center 1/3 process tube	0	0
end 1/3 process tube	0	0
spacer	3.2 E-05	3.1 E-11
connector	1.4 E-05	8.3 E-09
riser	7.2 E-10	5.5 E-10

Volume	Mass in/ (Mass in - Mass Condensed) ⁷	Mass in/ (Mass in - Mass Deposited as Aerosol) ⁷
center 1/3 process tube	1	1
end 1/3 process tube	1	1
spacer	3.3	1 + 6.8 E-07
connector	401	1 + 6.0 E-04
riser	1.5 E-05	3.0 E-07
net	1356	1 + 1.9 E-04

⁷The ratio $DF_{sum} = \text{mass in} / (\text{mass in} - \text{net mass removed})$ for a volume with several parallel methods of removal can be calculated from the relation

$$\frac{1}{DF_{sum}} - 1 = \sum_{i=1}^n \left(\frac{1}{DF_i} - 1 \right)$$

where DF_{in} is = mass in / (mass in - mass removed by i th means). Of course, direct application of the definition shows the DF_{sum} for series removal processes like one volume after the other is

$$DF_{sum} = \prod_{i=1}^n DF_i$$

when each DF_i represents all the removal processes at each step. However, the product formula is not applicable when DF_i represents only one of number of parallel processes.

TABLE 5.2. CALCULATED CsOH DISTRIBUTION AT 600 SECONDS

Mass released from uranium	2.19 E-04 kg
Mass chemisorbed	4.63 E-08 kg
Mass condensed	2.19 E-04 kg
Mass deposited as aerosol	2.69 E-08 kg

Volume	Mass Chemisorbed (kg)	Mass Condensed (kg)	Mass Deposited as Aerosol (kg)
center 1/3 process tube	0	0	0
end 1/3 process tube	0	0	0
spacer	0	1.5 E-04	1.3 E-10
connector	4.6 E-08	6.6 E-05	2.5 E-08
riser	5.7 E-12	3.6 E-09	1.8 E-09

Volume	Mass in / (Mass in - Mass Chemisorbed)	Mass in / (Mass in - Mass Condensed)	Mass in / (Mass in - Mass Deposited as Aerosol)
center 1/3 process tube	1	1	1
end 1/3 process tube	1	1	1
spacer	1	3.3	1 + 5.9 E-07
connector	1 + 7.0 E-04	244.	1 + 3.8 E-04
riser	1 + 2.8 E-05	1.02	1 + 9.3 E-03
net	1 + 2.1 E-04	815	1 + 1.2 E-04

TABLE 5.3. CALCULATED Te DISTRIBUTION AT 600 SECONDS

Mass released from uranium	7.92 E-06 kg
Mass chemisorbed	7.39 E-07 kg
Mass condensed	7.18 E-06 kg
Mass deposited as aerosol	3.18 E-10 kg

Volume	Mass Chemisorbed (kg)	Mass Condensed (kg)	Mass Deposited as Aerosol (kg)
center 1/3 process tube	2.6 E-07	0	0
end 1/3 process tube	2.5 E-07	0	0
spacer	8.2 E-08	5.0 E-06	0
connector	1.5 E-07	2.1 E-06	2.9 E-10
riser	5.3 E-11	5.1 E-11	2.5 E-11

Volume	Mass in / (Mass in - Mass Chemisorbed)	Mass in / (Mass in - Mass Condensed)	Mass in / (Mass in - Mass Deposited as Aerosol)
center 1/3 process tube	1.03	1	1
end 1/3 process tube	1.03	1	1
spacer	1.01	3.1	1
connector	1.07	14.3	1 + 1.3 E-04
riser	1 + 1.0 E-05	1 + 1.0 E-05	1 + 4.8 E-06
net	1.10	10.7	1 + 4.0 E-05

TABLE 5.4. CALCULATED SnTe DISTRIBUTION AT 600 SECONDS

Mass released from uranium	3.00 E-08 kg
Mass chemisorbed	0
Mass condensed	3.00 E-08 kg
Mass deposited as aerosol	1.49 E-12 kg

Volume	Mass Condensed (kg)	Mass Deposited as Aerosol (kg)
center 1/3 process tube	0	0
end 1/3 process tube	0	0
spacer	2.1 E-08	0
connector	8.6 E-09	1.4 E-12
riser	3.7 E-13	1.2 E-13

Volume	Mass in/ (Mass in - Mass Condensed)	Mass in/ (Mass in - Mass Deposited as Aerosol)
center 1/3 process tube	1	1
end 1/3 process tube	1	1
spacer	3.5	1
connector	297	1 + 1.6 E-04
riser	1.01	1 + 4.2 E-03
net	1050	1 + 5.0 E-05

TABLE 5.5. CALCULATED ZrO_2 DISTRIBUTION AT 600 SECONDS

Mass released	2.68 E-05 kg
Mass chemisorbed	0
Mass condensed	8.32 E-28 kg
Mass deposited as aerosol	2.64 E-05 kg

Volume	Mass Condensed (kg)	Mass Deposited as Aerosol (kg)
center 1/3 process tube	5.4 E-28	2.6 E-05
end 1/3 process tube	2.9 E-28	4.4 E-07
spacer	2.6 E-32	6.0 E-09
connector	9.8 E-33	1.0 E-07
riser	3.7 E-37	6.0 E-09

Volume	Mass in/ (Mass in - Mass Condensed)	Mass in/ (Mass in - Mass Deposited as Aerosol)
center 1/3 process tube	1 + 2.0 E-23	28.
end 1/3 process tube	1 + 3.1 E-22	1.9
spacer	1 + 5.1 E-26	1.01
connector	1 + 2.0 E-26	1.26
riser	1 + 9.3 E-31	1.02
net	1 + 3.1 E-23	67

separator and connector than the model predicts. Based on the interpretation of the LACE LA1 results, it is likely that this extra transport is due to resuspension and transport of deposited material along the surface so that the extra material would not be carried beyond the separator or upstream end of the connector where the fluid speed slows considerably. The author would expect to see a drift of this material at either the separator or the start of the connector where surface transport and resuspension become ineffective. By 600s, fluid speeds are down to 57 to 19 m/s so that conditions at the spacers and downstream volumes are more similar to the Power Burst Facility scoping test than the LACE LA1 test. Under these conditions, any error in the aerosol transport calculations is probably in the direction of an under-prediction of the aerosol deposition because of the omission of the pipe bend model.

Sensitivity studies in which the deposition velocity is arbitrarily reduced by a factor of three and in which the model for the effect of pipe bends is added were run to assess the effect of the uncertainty in the calculated aerosol deposition rate. The effect of these changes is discussed in Section 6.

5.2. Fission Product Behavior

It was mentioned earlier that the fission product species cesium iodide, cesium hydroxide, tellurium, and tin telluride are not sufficiently concentrated to form an aerosol on release from the fuel and that cooling by heat transport to walls is accompanied by vapor transport to walls at rates which discourage significant condensation on existing aerosols. The minimal role played by condensation onto the ZrO_2 aerosol in the base case is also due to the fact that the aerosol is deposited before the gas cools sufficiently to cause condensation onto the aerosols, as indicated in Tables 5.1 to 5.5. For all these reasons, aerosol behavior is not an important consideration in fission product behavior in the best estimate analysis of the N Reactor cold leg break.

The fact that the fluid does not cool sufficiently rapidly to cause condensation on aerosol seeds before their deposition does not mean that the gas remains much hotter than the wall. The time constants for the approach of the gas temperature to the wall temperature in the five volumes are greater than the time constants for vapor transport to the wall but still only 6.4×10^{-2} , 7.0×10^{-2} , 1.9×10^{-1} , 1.4×10^{-1} , and 1.5×10^{-2} s so the gas temperature follows the wall temperature fairly well as the pulse proceeds. The limited cooling of the gas in the process tube is due to the fact that there is no heat sink that lowers the temperature below saturation for the concentrations released until the gas arrives at volume 3, the separator part of the process tube. It follows that an increase in fission product release rates, a decrease in the source rates of diluting gases (steam and hydrogen), or a decrease in wall temperatures will all tend to cause more condensation of the fission product species. On the other hand, continued flow of very dilute gas will tend to cause revaporization from hot walls that contain condensed fission products and an increase in the wall temperatures of the separator or the connectors would prevent condensation in these volumes. A quantitative estimate of the effect of these variations is provided in Section 6.

In order to proceed with the discussion of fission product behavior it is useful to introduce time constants for chemisorbtion to the walls and for condensation/evaporation to the walls. This requires a discussion of the models used for condensation/evaporation and chemisorbtion.

The model for the transport of material to or from a reacting surface was developed by D. A. Powers³. It assumes mass transport acts in series with the parallel combination of condensation on the surface or chemical reaction with the surface. The gas phase mass transport rate is given by the following expression:

$$\frac{1}{A} \frac{dN(i)}{dt} = \frac{k_m}{R} \left[\frac{P_{bulk}}{T_{gas}} - \frac{P_{surf}}{T_{surf}} \right] \quad (5.1)$$

where

- R = the gas constant (Pa m³/(K kg-mole))
- N(i) = moles of species i transported to the surface
- P_{bulk}(i) = partial pressure of species i in the gas phase (Pa)
- P_{surf}(i) = partial pressure of species i in the close neighborhood of the surface (Pa) (determined with a steady-state assumption described later)
- T_{gas} = temperature of the gas (K)
- T_{surf} = temperature of the surface (K).

At the present time the TRAP-MELT2.0 expression for k_m in m/s is used

$$k_m = \frac{0.023 \text{ Re}^{0.8} \text{ Sc}^{0.33} D_v}{D_{ia}} \quad (5.2)$$

where

- Re = Reynold's Number, density speed Dia / viscosity
- Sc = Schmidt Number, viscosity /(density D_v)
- D_v = diffusivity of Tin vapor in steam (m²/s)
- and Dia = diameter of the pipe (m).

The rate of vapor condensation after transport across the gas boundary layer is assumed to be given by

$$\frac{1}{A_c} \frac{dN(i)}{dt} = k_c(i) [P_{surf}(i) - P_{eq}(i)] \quad (5.3)$$

where

- A_c = area available for condensation (m²)
- k_c(i) = condensation rate constant for species i (kg-mole/(kg m/s))
- P_{eq}(i) = equilibrium partial pressure of species i (Pa)

The rate of molecular bombardment is used for k_c²⁰

$$k_c(i) = \sqrt{\frac{1}{2\pi R} \frac{1}{M(i)T_{surf}}} \quad (5.4)$$

where

$M(i)$ = molar mass of species i (kg/kg-mole)

The rate of vapor reaction or reactant decomposition is calculated with the expression

$$\frac{1}{A_R} \frac{dN(i)}{dt} = \frac{k_R(i)}{RT} \left[P_{surf}(i) - P'_{eq}(i) \right] \quad (5.5)$$

where

A_R = area available for chemical reaction (m^2)
 $k_R(i)$ = reaction rate for species i (m/s)
 $P'_{eq}(i)$ = equilibrium partial pressure of species i over the product of the chemical reaction (Pa).

Empirical deposition velocities from TRAP-MELT are used for the reaction rates:

$$\text{for CsOH on stainless steel} \quad k_R = 1.0 \text{ E-04 m/s} \quad (5.6)$$

$$\text{for all CsI or CsOH on Zircaloy} \quad k_R = 0. \quad (5.7)$$

Also, P'_{eq} is assumed to be zero, thus not allowing any decomposition of the chemisorbed material.

In order to find $P_{surf}(i)$, it is assumed that steady-state conditions are valid at the surface region for any species:

$$\left. \frac{dN(i)}{dt} \right|_{\text{across gas layer}} = \left. \frac{dN(i)}{dt} \right|_{\text{condensing}} + \left. \frac{dN}{dt} \right|_{\text{reacting}} \quad (5.8)$$

Solution for $P_{surf}(i)$ yields

$$P_{surf}(i) = \frac{\frac{A k_m(i)}{RT_{gas}} P_{bulk}(i) + A_c k_c(i) P_{eq}(i) + \frac{A_R k_R(i)}{RT_{surf}} P'_{eq}(i)}{\frac{A k_m(i)}{RT_{surf}} + A_c k_c(i) + \frac{A_R k_R(i)}{RT_{surf}}} \quad (5.9)$$

In all of these calculations, the areas A , A_C , and A_R are assumed equal because the author has no data to indicate how these parameters may vary.

The models are cast in the usual form for evaporation/condensation calculations by converting the partial pressures in Equations (5.4) and (5.5) to concentrations using the ideal gas law:

$$P(i) = C(i) \frac{RT}{M(i)} \quad (5.10)$$

where $C(i)$ is the gas phase concentration of species i .

In order to define a time constant for evaporation/condensation, one sets k_R , the chemical reaction rate, equal to zero and finds from Equations (5.1), (5.9), and (5.10)

$$\frac{dC(i)}{dt} = - \frac{A}{V} \left[\frac{k_m(i) k_c(i) R T_{surf}}{k_m(i) + k_c(i) R T_{surf}} \right] [C(i) - C_{eq}(i)] \quad (5.11)$$

where

$C_{eq}(i)$ = the i th species equilibrium concentration just over a surface at T_{surf} (kg/m^3)

For constant T_{surf} and $C_{eq}(i)$, the solution of Equation (5.11) is an exponential curve with $C(i)$ approaching $C_{eq}(i)$. The time constant for this approach is

$$\frac{1}{\tau_c} = - \frac{A}{V} \frac{k_m(i) k_c(i) R T_{surf}}{k_m(i) + k_c(i) R T_{surf}} \quad (5.12)$$

where

τ_c = time constant for evaporation/condensation (s)
time for $C(i)$ to move $[1 - \exp(-1)] = 0.63$
of the way toward $C_{eq}(i)$

One can also define a time constant for chemisorption by considering rates for $k_C = 0$. In this case

$$\frac{1}{\tau} = - \frac{A}{V} \frac{k_m(i) k_R(i)}{k_m(i) + k_R(i)}$$

where

τ_c = time constant for chemisorption (s).

Comparison of the time constant and the average residence time of a slug is useful for interpreting calculations. In Table 5.6 these comparisons are displayed along with the area-to-volume ratios of the volumes. The table shows that the time constant for evaporation/condensation to the

TABLE 5.6. TIME CONSTANTS AND RESIDENCE TIMES AT 545 SECONDS

Volume	$\frac{A}{V}$ (m ⁻¹)	τ evap/cond. to wall (s)	τ chem CsOH (s)	τ chem Te (s)	τ resid. (s)
center 1/3 process tube	347.8	7.6 E-03	infinite ⁸	1.4	5 E-02
end 1/3 process tube	347.8	8.2 E-03	infinite	1.4	5 E-02
spacer	66.4	1.2 E-01	infinite	7.5	1.3 E-01
connector	79.5	8.6 E-02	1.3 E+02	1.3	6.2 E-01
riser	7.6	1.0 E+00	1.3 E+03	13.2	2.8 E-01

⁸The infinite time constants correspond to surfaces that have no chemisorption.

wall is less than the residence time in the process tube and connector tubes, about equal to the residence time in the spacer volume, and somewhat longer than the residence time in the riser where the surface-to-volume ratio is relatively low. This means that condensation to almost the equilibrium concentration at the wall temperature would occur in the process tube if gas concentrations were above the equilibrium concentration at the wall temperature. When the gas slug does encounter a region where the walls are cool enough to cause condensation of the fission product species, namely the spacer region in the best estimate analysis, the fact that the residence time is about equal to the time constant for condensation means that condensation will proceed $\approx 1 - e^{-1} \approx 0.63$ of the way toward equilibrium before the slug moves to the connector. The residence time is ten times the time constant for condensation in the connectors so condensation will proceed $\approx 1 - e^{-10} \approx 0.99995$ of the way toward equilibrium at the wall temperature of this volume. Very little additional condensation occurs in the risers because the residence time is only ≈ 0.25 times the condensation time constant and because the riser wall is not much cooler than the connector wall.

Condensation of fission products onto the ZrO_2 aerosol starts soon after condensation onto the wall because the gas temperature, and thus the temperature of the aerosol surface is not much hotter than the wall temperature. Thus Tables 5.1 to 5.5 show some fission products condensed on aerosols that later deposit on walls beginning in the spacer volume and increasing in the connectors where the aerosols have more fission product condensate.

With the exception of tellurium in the connector tube, the chemisorption constants shown in Table 5.6 are several times the residence times. This means chemisorption would remove most of the rapidly reacting tellurium species in the cross over tube if the species had not already condensed in the spacer or were not condensing at a rapid rate in the connector. This result is probably a little misleading because there is no model for chemical reaction of the condensed tellurium. It is the author's expectation that both the "chemisorbed" and "condensed" tellurium would be found in a reacted state with the spacer or connector metal. The slow reaction rate of the other species can be interpreted similarly. The chemical reaction of these species is much less effective than condensation at immobilizing the species but could cause a reaction in the condensed state that would affect possible revaporization.

6. EFFECT OF UNCERTAINTIES

As the best estimate or base-case analysis of fission product behavior in the N Reactor during a cold leg manifold break was developed, numerous uncertainties in the input data became apparent. This section is an assessment of the effects of these uncertainties.

The first uncertainty to be addressed is the length of the problem. It was recognized that the model for release from metallic fuel predicts a rapid release rate when the metal begins to oxidize and a slower rate when a protective oxide layer thickens. One would therefore expect that extending the analysis time span would cause little additional release from the fuel but condensation of a smaller fraction of the additional material released because of the low concentration of the additional material released. Section 6.1 shows the effect of extending the final time from 600 to 695 s and confirms the expectation that 600 s is sufficiently long to adequately define decontamination factors for the analysis.

It was also recognized during the analysis of the best estimate case that there is some uncertainty in the wall temperatures of the spacer region of the process tube and of the connectors. The effect of the uncertainty was investigated by raising the wall temperatures until they were hot enough to decrease the fractions of CsI, CsOH, and Te condensed. The results of these perturbations are discussed in Section 6.2. One can also exceed equilibrium concentrations by decreasing the coolant flow rate or increasing the rate of release of the fission products. These changes are investigated in Section 6.3, where the effects of multiplying the coolant flow rate by 0.1 and 5.0 are discussed, and in Section 6.4, where the effect of increasing the release rate (and the net release) by a factor of 10 is discussed.

The base case analysis suggests that the aerosol is not a significant contributor to fission product behavior. However, the rate of aerosol formation from structural materials is very uncertain so it is possible that significant changes could result from the very large changes in the source rates of a seed aerosol corresponding to the large uncertainty of the rate of aerosol formation. The effect of the uncertainty was tested by increasing the ZrO_2 aerosol source rate by factors of 10 and 100. The results are discussed in Section 6.5 along with the effects of multiplying the aerosol deposition velocity by 0.33, the correction suggested by the LACE LA1 test data, and activating the pipe bend model which was removed because it increased the difference between the calculated LA1 aerosol deposition and the test data.

Section 6.6 investigates the some of the effects of a change in the environment from pure steam to pure hydrogen. The final section, Section 6.7, investigates the impact of a change of the assumed initial geometric mean aerosol particle size. The investigation shows that formation of a very small initial aerosol size (a smoke rather than the droplet sizes generated in the LACE experiments) would increase fission product transport significantly.

6.1. Longer Problem Times

Table 6.1 is a summary of the effect of increasing the final time of the analysis from 600 s to 695 s. For cesium iodide and cesium hydroxide, there is some additional release at a relatively slow rate during the time span from 600 to 695 s but the fractions condensed and deposited change very little. For these species, the wall temperatures of the separator and downstream volumes represent such low equilibrium concentrations, C_{eq} , that the effect of the more dilute concentration on the rate of condensation given by Equation (4.1) is negligible. That is, the C_{eq} in the equation can be neglected compared to C and the rate of condensation predicted is proportional to the concentration so the fraction condensed is independent of the concentration. The tellurium results display a small effect due to the decreasing release rate. The fraction condensed decreases from 0.907 to 0.892. The reduction is more significant for tellurium because C is closer to C_{eq} for this species.

6.2. Increased Wall Temperatures

No reason for expecting higher wall temperatures has been identified but it was decided to define the increase required to prevent condensation by increasing the presumed wall temperatures until a significant change in condensation occurred. Figures 6.1 to 6.3 illustrate the effect of increases of the wall temperatures of the spacer, the connector, and the riser volumes by 100, 200, 250, and 300 K above the best estimate temperatures on the behavior of cesium iodide, cesium hydroxide, and tellurium. The figures show that an increase of 250 K is sufficient to prevent condensation of a significant fraction of the cesium iodide, while an increase of 200 K is sufficient to affect the condensation of cesium hydroxide. Tellurium condensation is affected by an increase of only 100 K but the fraction chemisorbed increases somewhat when less vapor is condensed and is therefore available to react chemically. When the wall temperatures are increased enough to prevent condensation of tellurium, the fraction chemisorbed becomes nearly independent of further increases in wall temperature at ≈ 0.4 of the tellurium released.

The behavior of cesium iodide is typical of that of cesium hydroxide and tellurium as wall temperatures increase. This behavior is illustrated in Tables 6.2 and 6.3 which show the distribution of cesium iodide when wall temperatures have been increased 200 and 250 K. Increases of 200 K prevent condensation in the spacer volume where most of the best estimate case condensation occurred. The spacers have become hot enough to keep the equilibrium concentration of cesium iodide at the wall temperature above the concentration of cesium iodide in the coolant. Because the time constant for condensation in the connector (shown in Table 5.6) is much shorter than the residence time, most of the cesium iodide is condensed in the first few sub-volumes of the connector and one sees an exponential "tailing off" of the amount condensed as he proceeds downstream in the connector. Subsequent condensation in the riser is limited in spite of the fact that it is cooler than the connector because the residence time in the riser is only about one fourth of the time constant for condensation and by the fact that the long residence time in the connector has reduced the vapor concentration to very near the equilibrium concentration at the temperature of the connector wall. Very little

TABLE 6.1. EFFECT OF INCREASING FINAL TIME FROM 600 TO 695 SECONDS

	600 Seconds final time		695 seconds final time	
	<u>(kg)</u>	<u>(fraction)</u>	<u>(kg)</u>	<u>(fraction)</u>
<u>CsI</u>				
released from uranium	4.57 E-05	1.000	5.50 E-05	1.000
condensed	4.56 E-05	0.998	5.49 E-05	0.998
deposited as aerosol	8.84 E-09	1.93 E-04	9.58 E-09	1.74 E-04
<u>CsOH</u>				
released from uranium	2.19 E-04	1.000	2.64 E-04	1.000
chemisorbed	4.63 E-08	2.11 E-04	5.81 E-08	2.20 E-04
condensed	2.19 E-04	0.998	2.63 E-04	0.996
deposited as aerosol	2.69 E-08	1.23 E-04	2.77 E-08	1.05 E-04
<u>Te</u>				
released from uranium	7.92 E-06	1.000	9.04 E-06	1.000
chemisorbed	7.39 E-07	0.093	9.59 E-07	0.106
condensed	7.18 E-06	0.907	8.06 E-06	0.892
deposited as aerosol	3.18 E-10	4.02 E-05	3.07 E-10	3.40 E-05

Figure 6.1. Effect of changes in wall temperatures on CsI behavior.

Figure 6.2. Effect of changes in wall temperatures on CsOH behavior.

Figure 6.3. Effect of changes in wall temperatures on Te behavior.

TABLE 6.2. CsI DISTRIBUTION WITH WALLS TEMPERATURES INCREASED 200 K

Mass released from uranium	4.57 E-05 kg
Mass chemisorbed	0
Mass condensed	4.39 E-05 kg
Mass deposited as aerosol	1.14 E-07 kg

Volume	Mass Condensed (kg)	Mass Deposited as Aerosol (kg)
center 1/3 process tube	0	0
end 1/3 process tube	0	0
spacer	0	0
connector	9.0 E-05	3.2 E-09
subvolume 1	4.26 E-05	0
subvolume 2	2.45 E-05	0
subvolume 3	1.14 E-05	0
subvolume 4	6.17 E-06	3.2 E-09
subvolume 5	2.96 E-06	0
subvolume 6	1.42 E-06	0
subvolume 7	7.00 E-07	0
subvolume 8	3.41 E-07	0
riser	9.8 E-07	7.1 E-11

TABLE 6.3. CsI DISTRIBUTION WITH WALLS TEMPERATURES INCREASED 250 K

Mass released from uranium	4.57 E-05 kg
Mass chemisorbed	0
Mass condensed	3.08 E-05 kg
Mass deposited as aerosol	5.87 E-12 kg

Volume	Mass Condensed (kg)	Mass Deposited as Aerosol (kg)
center 1/3 process tube	0	0
end 1/3 process tube	0	0
spacer	0	0
connector	3.1 E-05	0
subvolume 1	1.68 E-05	0
subvolume 2	8.30 E-06	0
subvolume 3	3.42 E-06	0
subvolume 4	1.29 E-06	0
subvolume 5	5.01 E-07	0
subvolume 6	2.07 E-07	0
subvolume 7	9.18 E-08	0
subvolume 8	4.37 E-08	0
riser	3.4 E-07	5.9 E-12

deposition on aerosols occurs because the equilibrium concentration at the gas temperature remains above the concentration until the fourth sub-volume. By this time, mass transport to the wall has reduced the amount of vapor significantly.

An increase of walls temperatures by 250 K produces a distribution similar to the distribution present when the walls temperatures were increased 200 K but with amounts reduced by a factor of three. No cesium iodide aerosol remains on the connector wall and the condensation on the cooler risers still does not dominate. At some point between 250 K and 300 K increases, the equilibrium concentration at the connector wall temperature would exceed the cesium concentration leaving the riser as the only site for condensation. The uncertainty study suggests that this occurs for only a very narrow range of temperatures.

An important result from this part of the uncertainty study is that condensation provides an upper limit to the rate of fission product transport of cesium iodide, cesium hydroxide, and tellurium. Increased concentrations in the fluid will be compensated by increased condensation. Another important observation is the fact that the wall temperature in the connector tube is the most important temperature to determine because the residence times are long compared to the time constants for condensation in this volume and the limiting equilibrium (shown in Figures 3.2 and 3.3) is a strong function of temperature.

6.3. Variations in Coolant Flow Rate

The effects of variations in coolant flow rate on the behavior of cesium iodide, cesium hydroxide, and tellurium are illustrated in Figures 6.4 to 6.6. The decrease of the fraction condensed on the wall for the case with the coolant flow in and out of the first volume reduced by a factor of 0.1 is caused by the increased fission product concentrations associated with the slower rate of diluting coolant flow. Because of the increased concentration, equilibrium concentration at the fluid temperature is exceeded and a very rapid condensation of the fission products onto the ZrO_2 aerosol occurs. Most of this aerosol is deposited in the spacer region but the smaller particles are transported beyond the riser, thus causing the counter-intuitive increase in the fraction that exits at the lower fluid flow rate. [The increase in material that exits is counter-intuitive because the rate of condensation onto both aerosols and the walls is increased by the increased concentration. One can see this by inspection of Equation (4.1). The mass transfer coefficient, k_w , which is approximately equal to the k_m of Equation (5.2) decreases in proportion to the speed to the 0.8 power because of the Reynold's number factor in k_m , but the residence time for the mass transfer to act is proportional to the speed to the -1 power. This means that the fractional decrease of $C - C_{eq}$ as a slug crosses a volume is nearly independent of the speed and one can estimate the changes in amount condensed by looking only at $C - C_{eq}$.]

6.4. Changes in Release Rates

Figures 6.7 to 6.9 illustrate the effect of order-of-magnitude increases in the rates of release of cesium iodide, cesium hydroxide, and tellurium

Figure 6.4. Effect of changes in coolant flow rate on CsI behavior.

Figure 6.5. Effect of changes in coolant flow rate on CsOH behavior.

Figure 6.6. Effect of changes in coolant flow rate on Te behavior.

Figure 6.7. Effect of an increase in the CsI and CsOH release rates on the CsI fractions condensed or deposited as aerosol.

Figure 6.8. Effect of an increase in the CsOH and CsI release rates on the CsOH fractions condensed, chemisorbed, or deposited as aerosol.

Figure 6.9. Effect of an increase on the CsI, CsOH, and Te release rates on the Te transport.

from the uranium fuel. The effect of this change is similar to the effect of the variations in coolant flow rate discussed in Section 6.3. The increased release rate causes the concentrations of the species to exceed equilibrium at both wall and gas temperatures in the upstream volume. This causes condensation on both aerosol and wall surfaces with a resultant increase in the amount deposited as aerosol and carried past the riser as an aerosol.

6.5. Variations in Initial Aerosol Source and Aerosol Deposition Rates

The effects of changes in either the low vapor pressure (ZrO_2) aerosol source rate or the rate of aerosol deposition on cesium iodide, cesium hydroxide, or tellurium behavior can be interpreted as changes in the surface area available for condensation. Since the temperatures and concentrations for the best estimate case are such that the equilibrium concentration at the gas temperature is barely exceeded, one would expect very little sensitivity to the amount of aerosol present.

Figures 6.10 to 6.12 show the changes in cesium iodide, cesium hydroxide, and tellurium behavior caused by increasing the ZrO_2 aerosol source rate by a factor of 10 and 100 (to one tenth the aerosol concentrations used in the LA1 experiment). Increasing amounts of aerosol increase the aerosol surface area and therefore the rate of condensation onto the aerosol so the fraction of both species deposited as an aerosol increases a little with increasing aerosol source rate. Condensation onto the wall is decreased because the vapor concentration is lowered more rapidly by the competing sink onto the aerosol and the fraction of each species that exits the standpipe is increased because many of the aerosol particles which contain condensate do not settle to the walls.

The effect of the uncertainties in the rate of removal of aerosols, shown in Figures 6.13 to 6.15, is similar to that of changes in the source rate. Reduction of the deposition rate by a factor of 0.33 increases the aerosol concentration in the connector and thus increases the fraction deposited as an aerosol because there is more aerosol surface area for fission product condensation. The fractional increase is less than that of Figures 6.10 to 6.12 because the uncertainty in the deposition rate is less than the uncertainty of the low volatility aerosol source rate.

6.6. Changes in Gas Composition

Figures 6.16 to 6.18 show that the effect of assuming a pure H_2 environment on the calculated behavior of cesium iodide, cesium hydroxide, and tellurium is minimal. This result is a little misleading because the model used for diffusion is not species dependent. The only way a change in majority species like steam or hydrogen can affect the calculated condensation, the major mode of fission product deposition for cesium and iodine, is by changing the gas density in the Reynold's number and Schmidt numbers in Equation (5.2). In reality, the change in the diffusivity of minority species as the majority component of the fluid changes could be the greatest effect of a change to a hydrogen environment. Also, a change in the H_2 to H_2O ratio could affect the chemical species formed by the elements present. The effect of a change in H_2 to H_2O ratio on the chemical species present is not modeled but a change in species could cause a significant change in fission product behavior.

Figure 6.10. Effect of increasing low vapor pressure aerosol source rate on CsI behavior

Figure 6.11. Effect of increasing low vapor pressure aerosol source rate on CsOH behavior.

Figure 6.12. Effect of increasing low vapor pressure aerosol source rate on Te behavior.

Figure 6.13. Effects of pipe bend deposition model and a factor of 0.33 reduction of the aerosol deposition rate on CsI behavior.

Figure 6.14. Effects of pipe bend deposition model and a factor of 0.33 reduction of the aerosol deposition rate on CsOH behavior.

Figure 6.15. Effects of pipe bend deposition model and a factor of 0.33 reduction of the aerosol deposition rate on Te behavior.

Figure 6.16. Effect of hydrogen concentration on CsI behavior.

Figure 6.17. Effect of hydrogen concentration on CsOH behavior.

Figure 6.18. Effect of hydrogen concentration on Te behavior.

6.7. Smaller Initial Aerosol Particle Volume

Figures 6.19 to 6.21 show the effect of reducing the assumed geometric mean particle volume of the initial aerosol to sizes smaller than those found in the LACE experiment. The reduced sizes include sizes characteristic of most smokes¹⁹. As one would expect, smaller aerosols are transported greater distances and can provide a condensation seed for the fission products.

Figure 6.19. Effect of variations in input geometric mean particle volume on CsI behavior.

Figure 6.20. Effect of variations in input geometric mean particle volume on CsOH behavior.

Figure 6.21. Effect of variations in input geometric mean particle volume on Te behavior.

7. CONCLUSIONS AND RECOMMENDATIONS

This section presents both preliminary implications for the N Reactor based on this fission product behavior analysis and recommendations for future analysis.

7.1. Preliminary Assessment of Implications for the N Reactor

The primary implication for the N Reactor deduced from this study is that most of the fission products remain in the molten uranium fuel. Only 0.033 of the hot-node, hot annular ring inventory is calculated to be released and this is only 0.0035 of the total inventory. If the release is controlled by fuel oxidation as available data suggest, longer times at temperature will not increase the release fraction significantly because the oxidation rate is proportional to the reciprocal of the oxide thickness. The small release is concentrated near the time the fuel cladding first ruptures and exposes the metal to steam but concentrations are still so low that condensation of the cesium and iodine species, cesium iodide and cesium hydroxide, does not begin until wall temperatures in the 700 to 800 K range are encountered. The corresponding temperatures for tellurium are 550 to 600 K but elemental tellurium reacts chemically in addition to condensing.

The description of the behavior of the cesium and iodide species relies on a defensible calculation of the wall temperatures in the process tubes and connector tubes because equilibrium concentrations are extremely sensitive to these temperatures. The vapor concentration that will be allowed to leave the risers increases about an order of magnitude for every 100 K increase in the wall temperature of the connectors. Because the best estimate temperatures of the spacers and connectors are on the order of 500 K, condensation plays a major role at the best estimate temperatures and for assumed temperatures up to 200 K higher than the best estimates. Another important parameter is the coolant flow rate. A reduction of the best estimate coolant flow rate by a factor of 0.1 increases fission product concentrations to the point that significant condensation onto pre-existing aerosols can occur. This, in turn, would allow transport of as much as half of some species of released fission products on the smaller aerosols. Formation of a very fine seed aerosol (a smoke) would also allow for transport of fission products as aerosols. Since no means of producing 700 to 800 K wall temperatures, a very fine seed aerosol or a factor of 0.1 reduction in coolant flow has been identified, decontamination factors are expected to be on the order of 1000 for CsI and CsOH.

Tellurium released from the molten uranium reacts rapidly with metal surfaces in the process and connector tubes but condensation in the spacer region is rapid enough to condense much of the tellurium in the spacer region before it reacts in the connector. This condensed material probably reacts with the surface after condensing but that reaction was not considered in this scoping study. Even when one ignores tellurium reactions, condensation provides a decontamination factor of ten for the best estimate calculation.

In the absence of species concentrations that significantly exceed equilibrium concentrations at the gas temperature (the best estimate

concentrations do not exceed the equilibrium), aerosol behavior is relatively unimportant in the analysis of the behavior of fission products in the cold leg manifold break scenario for the N Reactor. It is difficult to identify a source of low volatile aerosol and even if releases two orders of magnitude above best estimate are presumed, most of the aerosol is deposited before the very dilute fission products encounter temperatures cool enough to initiate condensation. For the large surface-to-volume ratios of the N Reactor, significant vapor transport is expected to the walls that provide a heat sink for the gas before the aerosol surface cools enough to be a condensation site for the cesium and iodine vapor species.

The best estimate calculation predicts 0.002 of the released cesium iodide, 0.002 of the released cesium hydroxide, and 0.001 of the released tellurium will be transported past the risers (mass released from the uranium/[mass released from the uranium - mass deposited] equal to 500, 500, and 1000, respectively). If these fractions are converted to absolute mass by multiplying by the inventories and the number of process tubes, 1003, one finds that the calculated releases past the risers are 9 E-05 kg of cesium iodide, 4 E-04 kg of cesium hydroxide, and 8 E-06 kg of tellurium.

7.2. Recommendations for Future Analysis

This scoping study has indicated that the transport of cesium and iodine fission product species is a strong function of wall temperatures in the process tubes and connector tubes. Particular care should be used to obtain accurate results for these parameters in any future analysis. It would also be desirable to assign an estimate of the uncertainty of this particular parameter. Coolant flow is also an important parameter, but the calculations are sensitive to this parameter only if flow is reduced enough (to a factor 0.1 times best estimate) to cause condensation onto pre-existing aerosols.

Since the metallic fuel is a significant barrier to the release of fission products, care should be taken to use this model correctly and make it defensible. Future analysis should use the non-isothermal version of the model. One improvement that would make the model easier to defend would be to cast the model for oxidation in terms of the rate of oxidation per unit surface area. However, this model improvement will only be useful if it can be used with an acceptable description of the surface area when the uranium fuel is first exposed to steam and during any subsequent relocation of the fuel.

The analysis tool used in this scoping study is unique because it calculates time constants for most mass transfer mechanisms. It is strongly recommended that future analysis with more sophisticated tools include the calculation of these time constants to aid interpretation of the results.

If future analyses are carried out to include behavior beyond the risers, a model for the solubility of cesium iodide and cesium hydroxide in condensed steam or water from any other source should be included. Water has been shown to be a very important parameter in the release and transport of cesium and iodine from reactors²¹.

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APPENDIX A - SUPPLEMENTAL THERMAL ANALYSIS

Table A.1 is a copy of the results of a supplemental analysis to determine the temperatures of the spacer tube, connectors, and risers.

TABLE A.1. TEMPERATURES OF SPACERS, CONNECTORS, AND RISERS

NOTEGRAM

To: Don Hagrman

Date: April 22, 1987

From: Steve Wagoner *SW*

BOUNDARY CONDITIONS FOR FISSION PRODUCT BEHAVIOR ANALYSIS

This notegram is in response to your request for wall temperatures in the spacer, the connector, and the riser regions. The temperatures provided are for a 200% cold leg manifold break without ECCS or GSCS. The temperatures are for a time appx 700 s. after break initiations. Peak fuel temperature at this time is 2000°F. The range in the values reflect the temperature gradient from the top to the bottom of the reactor.

<u>LOCATION</u>	<u>TEMPERATURE (°F)</u>
Spacers	580 - 600
Connectors	430 - 475
Risers	405 - 470

These calculations have not been reviewed and therefore would still be considered preliminary. If you have further questions please call me on FTS 444-9219.

cc: J Martin
S Heaberlin

APPENDIX B INPUT REQUIREMENTS FOR ANALYSIS TOOL

Table B.1. is a list of the input requiremnts for the analysis tool used to study fission product behavior in the N Reactor.

TABLE B.1. INPUT REQUIREMENTS FOR PULSE

1. NV NV = number of major (boundary
110 conditions specified) control
 volumes.
2. NSV(I) NSV(I) = number of sub-volumes in
2014 I th control volume
3. Z(I), AC(I), AW(I), ASET(I), IWALL(I) Z(I) = volume length (m)
NV*(4E10.3,110) AC(I) = flow channel cross
 sectional area (m)
 AW(I) = Wall surface area (m)
 ASET(I) = Component of wall surface
 normal to acceleration of
 gravity (m)
 IWALL(I) = wall composition
 0 = zircaloy
 1 = stainless steel
4. BENDR(IS) BENDR(IS) = angle through which pipe bends
NSV(I)*(8E10.3) in IS th subvolume (radians)
5. TIMEI, TIMEF TIMEI = time at start of problem
2E10.3 TIMEF = time at end of problem
6. ISPC(K) K=1,20 ISPC(K) = switch indicating whether K th
2014 species is to be considered
 K = 1 for iodine
 K = 2 for cesium iodide
 K = 3 for cesium hydroxide
 K = 4 for tellurium
 K = 5 for cadmium
 K = 6 for silver
 K = 7 for strontium hydroxide
 K = 8 for barium hydroxide
 K = 9 for hydrogen telluride
 K = 10 for hydrogen iodide
 K = 11 for tin
 K = 12 for tin telluride
 K = 13 for water vapor
 K = 14 for zirconium dioxide
 K = 15 for uranium dioxide
 K = 16 for carbon
 K = 17 for XX
 K = 18 for XY
 K = 19 for XZ
 K = 20 for YX
 set = 0 for do not consider,
 1 for consider
7. TOL1, TOL2 TOL1 = fractional tolerance allowed on states
2E10.3 with enough mass to be considered
 TOL2 = minimum state mass considered (kg)

TABLE B.1. INPUT REQUIREMENTS FOR PULSE (CONTINUED)

8. IPSKIP, IPS
2I10

IPSKIP = print frequency control
 IPSKIP = 0 to print only final state
 = 1 to print after each pulse
 = 2 to print after every
 second pulse
 = 3 to print after every
 third pulse

IPS = print information control
 IPS = 0 to print input echo,
 deposition at end of problem,
 packet and volume number
 IPS = 1 to print IPS = 0 information
 plus subvolume-by-subvolume
 concentration at end of problem
 IPS = 2 to print IPS = 1 information
 plus subvolume-by-subvolume
 concentration before and after
 pulse, total amount of species
 input, amount of species out of
 last volume, mass accounted for
 IPS = 3 to print IPS = 2 information
 plus pulse concentration, amount
 condensed on wall, chemisorbed on
 wall, vapor temperature, wall
 temperature, pulse volume, vapor
 velocity, vapor pressure,
 equilibrium vapor concentration,
 volume and wall heat sources,
 packet number, subvolume number,
 time, amount of aerosol on wall
 IPS = 4 to print IPS = 3 information
 plus species mass distribution
 among aerosol states, particle
 number distribution among aerosol
 states, time constant for
 vapor-to-aerosol
 evaporation/condensation
 IPS = 5 to print IPS = 4 information
 plus volume heat source, pulse
 center transit time, time constant
 for vapor-to-wall
 condensation/evaporation
 IPS = 6 to print IPS = 5 information
 plus particle deposition
 velocities, increase in effective
 wall temperature due to gas
 heating, timeconstants for aerosol
 deposition, bin shift due to
 evaporation/condensation,
 agglomeration out of bins, and gas
 temperature change

TABLE B.1. INPUT REQUIREMENTS FOR PULSE (CONTINUED)

9. a) FPISO(IRE), IRE=1,5 5E10.3	FPISO(IRE) = mass fraction of chemical element consisting of given isotope
b) FPISO(IRE), IRE=6,11 6E10.3	IRE = 1 for Cesium 133
c) FPISO(IRE), IRE=12,16 5E10.3	IRE = 2 for Cesium 134
d) FPISO(IRE), IRE=17,23 6E10.3	IRE = 3 for Cesium 135
e) FPISO(IRE), IRE=24,28 5E10.3	IRE = 4 for Cesium 137
	IRE = 5 for Cesium 140 (end of first card)
	IRE = 6 for Iodine 127
	IRE = 7 for Iodine 131
	IRE = 8 for Iodine 132
	IRE = 9 for Iodine 133
	IRE = 10 for Iodine 135
	IRE = 11 for Iodine 137 (end of second card)
	IRE = 12 for Krypton 85
	IRE = 13 for Krypton 85M
	IRE = 14 for Krypton 87
	IRE = 15 for Krypton 88
	IRE = 16 for Krypton 90 (end of third card)
	IRE = 17 for Tellurium 129M
	IRE = 18 for Tellurium 130
	IRE = 19 for Tellurium 131
	IRE = 20 for Tellurium 131M
	IRE = 21 for Tellurium 132
	IRE = 22 for Tellurium 133
	IRE = 23 for Tellurium 135 (end of fourth card)
	IRE = 24 for Xenon 133
	IRE = 25 for Xenon 133M
	IRE = 26 for Xenon 135
	IRE = 27 for Xenon 137
	IRE = 28 for Xenon 140

Note: All fractions corresponding to the elements of chemical species are to be input. For example, If no species containing Cesium is indicated in item 6, item 9 a should still be present.

TABLE B.1. INPUT REQUIREMENTS FOR PULSE (CONTINUED)

Note: Items 10 and 11 are repeated for each species

10. a) NJS(KR) NJS(KR) = number of time-vapor rate pairs
I10 for KR th considered species source
- b) TSPEC(KR,J),RSPEC(KR,J),J=1,NJS(KR)
2E10.3 TSPEC(KR,J) = time part of time-vapor source
rate table for KR th considered species
source (s)
RSPEC(KR,J) = source rate part of time-
vapor source rate table for the KR th
considered species source (kg/s)
11. a) IATYP IATYP = switch indicating the type of
I10 aerosol source rate input
0 = input will be geometric mean
volume, geometric standard
deviation based on volume, and
total aerosol mass rate for the
species
1 = input will be mass rate bin-by-bin
for the current species
2 = No aerosol of the current species
will be input

Case I: IATYP = 0

- b₁ NJA(KR) NJA(KR) = number of time-aerosol parameters
I10 table entries
- c₁ TAERO(KR,J),XBAR(KR,J),SIG(KR,J),RMAS(KR,J),J=1,NJA(KR)
4E10.3 TAERO(KR,J) = time part of time-aerosol
parameters table for KR th
considered species (s)
XBAR(KR,J) = geometric mean particle volume
part of time-aerosol parameters
table of KR th considered
species (m³)
SIG(KR,J) = geometric standard deviation
based on volume part of
time-aerosol parameters table for
KR th considered species
RMAS(KR,J) = total aerosol mass rate for
the species part of time-aerosol
parameters table for KR th
considered species (kg/s)

Case II: IATYP = 1

- b₂ NJA(KR) NJA(KR) = number of time-bins source rates
I10 table entries
- c₂ TAERO(KR,J),J=1,NJA(KR) TAERO(KR,J) = time part of time bins sources
//2X,4E10.3 rate pairs (s)
- d₂ RAERO(KR,L,J)L=1,20,J=1,NJA(KR) RAERO(KR,L,J) = aerosol mass rate
8E10.3 into the L th bin for KR th species
(kg/s)

CASE III: IATYP = 2
No additional input

TABLE B.1. INPUT REQUIREMENTS FOR PULSE (CONTINUED)

12. a) NJF
I10 NJF = number of time-gas source rates and time-gas composition pairs
- 12 b) and 12 c) repeat for J = 1 to NJF
b) TFLOW(J),RFLOW(J),GMIX(1,J),GMIX(2,J)
4E10.3 TFLOW(J) = time part of time-gas mass rate and time-gas composition tables (s)
RFLOW(J) = gas mass rate part of time-gas mass rate table (kg/s)
GMIX(LCI) = molar fraction of LCI th gas component part of time-molar fraction of LCI th gas component table (unitless)
LCI = 1 is helium
LCI = 2 is argon
LCI = 3 is krypton
LCI = 4 is xenon
LCI = 5 is hydrogen
LCI = 6 is nitrogen
LCI = 7 is oxygen
LCI = 8 is carbon monoxide
LCI = 9 is carbon dioxide
LCI = 10 is water vapor
- c) GMIX(LCI,J),LCI=3,10
8E10.3
- Note: these gases are presumed to be non-condensable
13. a) NJGT
I10 NJGT = number of time-input gas temperature pairs
b) TGTMP(J),GTMP(J),J=1,NJGT TGTMP = time part of time-input gas temperature table (s)
2E10.3 GTMP(J) = input gas temperature part of time-input gas temperature table (K)
14. a) NJWT
I10 NJWT = number of time-wall temperature pairs for table describing each main volume
- 14 b) repeats for each main volume
b) TWTMP(I,J),WTMP(I,J),J=1,NJWT NJWT = number of time-wall temperature pairs for table describing each main volume
2E10.3 TWTMP(I,J) = time part of time-wall temperature table for I th volume (s)
WTMP(I,J) = wall temperature part of time-wall temperature table for I th main volume (K)

TABLE B.1. INPUT REQUIREMENTS FOR PULSE (CONTINUED)

15. a) NJGP I10	NJGP = number of time-input gas pressure pairs
b) TGPRS(J),GPRS(J),J=1,NJGP 2E10.3)	TGPRS(J) = time part of time-input gas pressure table (s) GPRS(J) = input gas pressure part of time-input gas pressure table (Pa)
16. a) NJTC I10	NJTC = number of time-boundary conditions time constant pairs
b) TTCBC(J),TCBC,J=1,NJTC 2E10.3	TTCBC(J) = time part of time-boundary conditions time constant table (s) NJTC(J) = boundary conditions time constant part of time-boundary conditions time constant table (s)
17. IBUG I10	IBUG = debug print-out switch IBUG = 0 for no debug print-out IBUG 1 for debug print-out

APPENDIX C - REVIEWER'S COMMENTS

This report has received independent technical review by M. Epstein of Fauske & Associates, Inc. and the reviewer's comments are reproduced as the remainder of Appendix C.

Fauske & Associates, Inc.

DATE: January 6, 1988

TO: William Quapp, Westinghouse Hanford Company

FROM: Michael Epstein, Fauske & Associates, Inc. M.E.

SUBJECT: Comments on "A Scoping Study of Fission Product Transport From Failed Fuel During N Reactor Postulated Accidents" by D. L. Hagrman

The author's main goal was to produce a scoping study that identifies the key areas relative to fission product behavior during an N Reactor severe accident. His report succeeds in this endeavor. However, there are several major technical points which the author should consider. Some of these comments may impact on the conclusions given in the executive summary. Moreover, we found it difficult to assess the correctness of the calculations, given the assumptions, because the report is somewhat unclear on methods and disorganized in presentation of data.

Major Problems

1. On page 20 the author rules out the possibility of CsI and CsOH aerosol formation on the basis that cooling by heat transport to walls is accompanied by an equivalent rate of vapor transport to walls. On the contrary, this is one situation that is conducive to aerosol formation. The rates of transport are not important; it is only the temperature "level" of the cold wall for a given free stream vapor concentration that determines the potential for aerosol formation. For the conditions given in the report it does not seem likely that the CsI or CsOH vapor species will be transported to the cold walls by vapor phase diffusion. Instead a zone of supersaturation will occur within the thermal boundary layer (Figure 1). If excessive local supersaturations are achieved, heterogeneous or homogeneous nucleation of aerosol within the

gaseous phase will occur, thereby influencing the overall fission product transport process. Note, from Figure 1, that aerosol formation is possible even for superheated (undersaturated) free stream conditions. Based on calculated release rates of 10^{-5} kg s^{-1} and 10^{-2} kg s^{-1} for CsOH and H_2O , respectively, we estimate a CsOH vapor pressure of 12 Pa. The equilibrium vapor pressure of CsOH at the spacer region wall temperature of 507K is 5.07×10^{-4} Pa. With these figures in mind, assuming that the Lewis number of the gas mixture is nearly unity, we predict a supersaturation of 52 in the cooler part of the boundary layer where the temperature has decreased to 600K. Typically, vapors in "laboratory clean" gases can not sustain supersaturations in excess of ~ 10 before homogeneous nucleation to an aerosol becomes inevitable. In practice, aerosol formation occurs at much lower supersaturations. Thus, it would appear that the vapor species transport model used in the report must be replaced by an aerosol transport and deposition model in order to properly evaluate fission product retention. The executive summary should be revised to reflect this situation indicating that aerosol transport is of primary importance and that the degree of fission product retention depends on the outcome of future studies that account for aerosol formation.

2. Results for fission product release and chemical form are very much governed by the assumptions. These assumptions and their impact are:
 - a. Metal fuel oxidation law (pp. 14 and 15). Determines the release fraction and CsI ratio. This law is not valid for degraded geometry.
 - b. Hydrogen to oxygen ratio H/O, assumed low but never stated (p. 13). For U-UO₂ equilibrium which is consistent with the stagnant flow assumption, this ratio is near or above 10^4 . This affects fission product release rates and chemical form.

- c. SnTe is assumed, and its presence is questionable but possible and needs defense.
- d. "Frozen" chemical form. Fission product chemical form, as released from fuel, need not be the same as that in the stagnant gas above the fuel, and chemical forms in other N Reactor control volumes need not be the same as those in the pressure tubes.

These assumptions impact on the conclusions given in the executive summary in the following ways.

- i. The potential for HI formation exists in the fuel channels, where uranium fuel may be oxidizing. However, in cooler regions and regions in which effluent mixing occurs, CsI will be the dominant form.
 - ii. Ru release is believed to be greatly overstated.
 - iii. Sr release from fuel will be sensitive to the fuel temperature, but high retention is expected.
3. The mode of deposition is governed by the core source rate. Using the same model of fission product release, Cronenberg [1] obtained different source rates than those predicted in this report for similar conditions. These differences should be resolved.

Minor Point

- 1. It is difficult to believe that interfacial resistance to condensation, as expressed by Equation (5.3), is important. Conditions at the surface of the condensed film should be well represented by the assumption $P_{\text{surf}} = P_{\text{eq}}$.

Reference

1. A. W. Cronenberg, "Scoping Analysis of Fission Product Behavior and Transport in the Primary Coolant System for Postulated N Reactor Severe Accidents", Unpublished Westinghouse Report, (August, 1987).

Figure 1 Vapor pressure and temperature profiles near a cold surface, demonstrating aerosol formation due to the attainment of supersaturation.

APPENDIX D - AUTHOR'S RESPONSE TO COMMENTS

This report has received independent technical review reproduced in Appendix C. The author's response is reproduced as the remainder of this appendix.

January 12, 1988

Dr. D. B. Bechtold
Westinghouse Hanford Company
Box 1970
Richland, WA. 99352

RESPONSE TO COMMENTS ABOUT EGG-7899 - DLH - 1 - 88

Dear Dr. Bechtold:

In our conversation of last December with you and W. J. Quapp, you requested that the INEL respond to the review comments of Fauske & Associates Inc. regarding the EG&G report EGG-SSRE-7899. I have reviewed the comments with cognizant personnel at the INEL and prepared the attached response that I hope you will find useful for planning your future analysis.

An additional potential problem that was not directly pointed out by Fauske and Associates Inc., is the lack of a description (user's manual) or verification of the analysis tool that was used. The tool is an adaptation of the TRAP-MELT2 computer code developed at Battelle Columbus by Hans Jordan, James A. Gieseke, and M. R. Kuhlman to the non-well mixed volumes (slug flow) we encountered in the analysis of some Power Burst Facility experiments. We have never been funded to write a code description or to carry out a complete verification of the models. However, I suspect that some sort of supporting documentation will be required at some point in your work.

If you have any questions, please contact me at FTS 583-9513.

Very truly yours,

D. L. Hagrman

Attachment:
As Stated

cc: G. A. Berna, DOE-ID
W. J. Quapp, WHC

Idaho, Inc.

P.O. Box 1625

Idaho Falls, ID 83415

RESPONSE TO FAI COMMENTS ABOUT EGG-SSRE-7899,
A SCOPING STUDY OF FISSION PRODUCT TRANSPORT FROM
FAILED FUEL DURING N REACTOR POSTULATED ACCIDENTS

D. L. Hagrman

Major points of the FAI review included questions about aerosol formation and fission product chemical form. I agree that the question of aerosol formation mentioned as major problem 1 in the FAI letter is not closed by the INEL report. D. A. Petti and I proposed additional work to investigate aerosol formation in to R. J. Dallman's letter to W. J. Quapp of November 30, 1987¹. However, I am not yet convinced that the mechanism of aerosol formation within the thermal boundary layer proposed by FAI is important or that other aerosol sources are not more important. There are two reasons for my reservation about the formation mechanism proposed by FAI:

- 1). They may have assumed that hot effluent above the fuel is transported suddenly to regions with cold walls. I don't know what fluid temperature and concentrations were used to calculate the supersaturation in the boundary layer mentioned in the review² of the INEL paper, but I noted a bulk temperature of 1370 K used in conjunction with the calculation of that result for the Cronenberg paper². That temperature is much too high for the geometry and flow of the N Reactor problem I analysed. I found that the gas cools to 980 K before the first wall temperature of 507 K is encountered and that the gas temperature drops to 720 K as the section of wall at 507 K is passed. Also, there is vapor condensation on the hotter walls upstream from the 507 K walls as the gas cools. This condensation begins as soon as saturation occurs (at wall temperatures) and may serve to keep vapor concentrations too low to nucleate significant aerosol.
- 2). Even if an aerosol does form near the wall, our staff suspects thermophoresis will cause most of it to deposit on the wall. If a model for transport of the aerosol formed in the boundary layer is what is meant by the statement, "it would appear that the vapor species transport model used in the report must be replaced by an aerosol transport and deposition model in order to properly evaluate fission product retention," I would agree that this model should accompany any model for aerosol formation in the boundary layer.

In order to help resolve aerosol formation questions, I would suggest that FAI perform improved calculations using spatially varying gas temperatures and fission product concentrations expected in the N Reactor to better show the need for these models. If it can be shown that this source is a major aerosol source, it would make sense to add the boundary layer aerosol formation model to all calculations.

The questions about the chemical form of the fission product species raised as point two in the FAI review were addressed as items (1) and (2) in the attachment to the November 30, 1987, letter mentioned earlier.

At the present time I am completing an equilibrium vapor chemistry model to be added to the tool used in the N Reactor analysis. I suspect that the principal effects of this additional modeling will be (1), the addition of minority fission product species "fed" by reactions of the majority species like

and (2) perhaps some temporal variations in the majority fission product species ratios with time. I expect this effect to be moderated by the short duration of the fission product release from the fuel if such short durations are still expected.

REFERENCE

1. R. J. Dallman letter to William Quapp, November 30, 1987
2. Robert E. Henry letter to William Quapp, December 4, 1987.